BEMScript for MERRILL 1.3.3

Documentation

Karl Fabian December 4, 2014

(additions by W Williams June 1 2018)

The script is a simple ASCII file containing a sequence of lines. Empty lines, leading, trailing, and multiple spaces or tabs are ignored, as well as anything behind an exclamation mark (!). A number of keywords are used to call subroutines or perform simple assignments. All keywords are case insensitive, e.g. 'ReadMesh' and 'readmesh' are equivalent. The script file is parsed line by line. Each valid line is immediately evaluated and executed.

The following list contains the currently available commands:

Set ⟨**variable**⟩⟨**value**⟩ is used to define global variables for the material, the geometry of the mesh, or program parameters. The following **variables** are supported:

Ms saturation magnetization in A/m.

K1 anisotropy constant for uniaxial or cubic anisotropy in J/m^3.

Aex exchange constant in J/m.

Ls inverse length scale 1/m. Internally Ls^2 is used.

mu related to permeability of free space via mu = $\mu 0/4\pi$.

NEBSpring Spring constant for nudged-elastic band method (NEB) .

CurvatureWeight Weight of curvature contribution for nudged-elastic band method (NEB) .

MaxMeshNumber Maximal number of finite element meshes stored. Must be set once before loading meshes.

PathN Number of structures along the magnetization path. Warning: The mesh must have been defined previously! Use only after ReadMesh.

ExchangeCalculator Chooses the exchange energy discretization method used. The available choices are 1= $m\,\Delta m$, 2= ϕ^2 along edges, 3= $(\nabla\vartheta)^2$ + $\sin^2\vartheta$ $(\nabla\phi)^2$.

MaxRestarts Maximum number of restarts during energy minimization.

MaxEnergyEvaluations Maximum number of energy calculations during energy minimization (typ- ical: 10000). Afterwards energy minimization is aborted.

MaxPathEvaluations Maximum number of path energy calculations during path minimization (typ- ical: 2000).

Zone Current Zone to be written into the TecPlot output file (double). Zone can be set before each output, or can be used with automatic increment.

ZoneIncrement Automatic increment of zone (default=1.0).

Magnetite ⟨**temperature**⟩ **C** Defines material constants for magnetite at temperature ⟨temperature⟩ to be used in subsequent calculations. The temperature is given in degrees Celsius and must be positive and below magnetite's Curie temperature at 580° C.

Resize ⟨**old length**⟩⟨**new length**⟩ changes the length scale of the mesh such that after this rescaling the length ⟨old length⟩ will become ⟨new length⟩ .

(cubic | uniaxial) anisotropy Defines the symmetry of the anisotropy energy.

CubicRotation <phi> <theta> <alpha>. Performs a 3D rotation of the cubic anisotropy axis. Variables are real numbers that specify the rotation angles in radians.

Optionally (not thoroughly tested) specify 4 variables <phi> <theta> <alpha> <Material Number>, where <Material Number > is an integer that applies to rotation to a specified material of a multi-phase model.

Easy axis ⟨*x*,*y*,*z*⟩ Determines the easy axis for uniaxial anisotropy.

External field direction ⟨*x*,*y*,*z*⟩ Determines the direction vector of an external homogenous magnetic field. Intrinsically sets the field to B = 1 T.

External field strength ⟨*B*⟩ , ⟨*unit*⟩ Determines the strength of the external homogenous magnetic field as B in units of unit. Possible values for unit are 'muT', 'mT', or 'T'. Must be set after defining the direction. Subsequent calls reset the field to B without changing the direction. Can be used for hysteresis modeling.

ReadMesh ⟨**index**⟩⟨**filename** ⟩ Reads the Patran file ⟨filename⟩, and stores the corresponding mesh and finite element arrays at location ⟨index⟩. The index must be less or equal to the previously set MaxMeshNumber.

LoadMesh ⟨**index**⟩ Loads a previously read mesh and its finite element arrays from location ⟨index⟩.

This mesh will then be used in subsequent operations.

ReadMagnetization ⟨**filename**⟩ Reads a magnetization file (.dat or .restart) into the current mesh magnetization array. Make sure that it was created for the currently active mesh! The magnetization read is used in subsequent operations.

Uniform magnetization ⟨*x*,*y*, *z*, [*b*] ⟩ Creates a uniform magnetization for the current mesh pointing in the normalized direction ⟨*x*,*y*,*z*⟩. The optional parameter b is the index of the block of nodes in the mesh that should be set. By definition block 1 contains the free nodes, while higher block numbers can be used to define fixed nodes. These block have to be defined in the Patran file. Any previous magnetization is lost!

Randomize magnetization ⟨*angle*⟩ Randomly changes each current magnetization vector by at most ⟨*angle*⟩ degrees. The previous magnetization is (partly) lost!

Randomize all moments Replaces the current magnetization by randomly distributed unit vectors. Any previous magnetization is lost!

ReMesh ⟨**index**⟩ Takes the current magnetization array and interpolates it at the nodes of the previously read mesh at location ⟨index⟩. This mesh from location ⟨index⟩ is then loaded and will be used in subsequent operations.

ConjugateGradient Uses conjugate gradient steps during the accelerated descent.

SteepestDescent Uses normal gradient steps during the accelerated descent.

Minimize Calls the minimization routine for the current mesh and initial magnetization. This call does not save the final result!

EnergyLog ⟨**filename**⟩ Starts logging all subsequent energy calculations into the logfile ⟨filename⟩.log. Logging can be stopped by *EndLog* or *CloseLogfile*

CloseLogfile ends the previous logging of energy calculations or path minimizations.

WriteMagnetization ⟨**filename**⟩ Saves the magnetization and the mesh in three files:

> ⟨**filename**⟩**.dat** contains vertex coordinates and magnetization vectors.
>
> ⟨**filename**⟩**.restart** same as the previous one (obsolete?).
>
> ⟨**filename**⟩**_mult.dat** TecPlot file for visualization using ParaView or TecPlot. Contains mesh geometry and one or more magnetization states.

WriteHyst ⟨**filename** ⟩ Saves hysteresis data in 5 columns of **M•H_ext , |H|** and the 3 components on the average unit M vector, where **M** is the magnetization and **H_ext** is the external field. **M•H_ext** is normalized to the saturated magnetization in the direction of the applied field. Output file is ⟨**filename** ⟩.hyst

WriteBoxData ⟨**filename** ⟩ Writes the magnetization per node along with the node associated volume x,y,x, m_x,m_y,m_z, vbox. Where x,y,x is the node location, m_x,m_y,m_z is the magnetization unit vector components, and vbox is the volume associated with a node (in units of microns^3). This is useful if you want to compute the absolute magnetization associated with each node.

MagnetizationToPath ⟨**index** ⟩ Saves the current magnetization in the path at location ⟨index⟩. This allows to assemble a path from individual magnetization states that have to fit to the current mesh! After assembling a path it must be renewed before further operations can be performed.

PathToMagnetization ⟨**index**⟩ Moves the path magnetization state at location ⟨index⟩ to the current magnetization. This allows to change individual magnetizations in the path. E.g. Initial and final states of a path read from a file can be minimized for new material constants.

RenewPath Defines all path variables, like distances and tangent vectors, assuming that all magnetizations have been correctly filled.

RefinePathTo ⟨newlength ⟩ Refines the current path to a new number of states by linear interpolation in the magnetization angles. This also resets *PathN* to the new value and renews the path. Of course, the new number of states can also be less than the previous *PathN* .

WriteTecPlotPath ⟨filename ⟩ Exports the current path to a TecPlot file with name ⟨filename ⟩ . All states along the path are individual zones in the TecPlotFile.

ReadTecPlotPath ⟨filename⟩ Reads a new path from a TecPlot file with name ⟨filename⟩ . All states along the path are individual zones in the TecPlotFile. Because this also reads in the mesh, all mesh related quantities are recalculated. Make sure that all material parameters are correctly assigned, since those are not read !

ReadTecPlotZone ⟨filename⟩ <zone number> Reads one zone from a TecPlot file with name ⟨filename⟩ and makes this the current magnetization. Can be used to read in an initial guess or as a start/end point of an initial path for NEB calaulations. No mesh information is read so make sure the mesh appropriate to the data is already loaded.

KeyPause Pauses script evaluation and waits for Key+Enter for continuation.

MakeInitialPath Assumes that a path is defined by *set PathN ⟨number ⟩* and that the first and last magnetization patterns are defined. Then proceeds by stepwise minimization to construct an initial path for subsequent optimization by the NEB method.

PathMinimize Assumes that an initial path is defined and minimizes the action integral using a variant of the NEB method.

PathLogfile ⟨filename ⟩ Starts logging all subsequent path minimization calculations into three logfiles ⟨filename ⟩ .enlog ⟨filename⟩.grlog, and ⟨filename ⟩.dlog. They contain energies along the path, norms of the gradients along the path and cumulative distances along the path. Logging can be stopped by *EndLog* or *CloseLogfile*.

SystemCommand ⟨command ⟩ ... Performs the system command in the remaining arguments as a line. No guarantee can be given for correct behavior. Uses FORTRAN's SYSTEM command.

PathStructureEnergies <filename> Computes the energies for each structure along the minimum energy path. The output is written to <filename>, however if this is omitted then the output is written to standard out.

ReportEnergy Makes a report on the model parameters (mesh size, material parameters, exchange length etc, as well as the component and total magnetic energy both in reduced units of (Kd. V) and in Joules.

(Stop | End) Stops script evaluation.

The following commands are advanced options for scripts using loops or variables. They are not thoroughly tested.

Loop ⟨**variable** ⟩ ⟨**startvalue** ⟩ ⟨**endvalue** ⟩ [⟨**step**⟩] Takes all commands until the next EndLoop statement and performs a loop over the enclosed commands by replacing the variable ⟨ variable⟩ with values from ⟨startvalue ⟩ to ⟨endvalue ⟩ in steps of ⟨step ⟩. If step is not given stepsize *step=1.0* is assumed. Within the loop the string #⟨variable⟩ is replaced by the integer value of variable, the string %⟨variable⟩ is replaced by the double precision value of variable , and the string $⟨variable⟩$ is replaced by a string of the value of variable . Nested loops are not supported! Warning: The *Loop* command itself must NOT contain variables! This is so because currently the parsing for replacing variables is performed only after unravelling the loops.

EndLoop Delimits the set of commands inside the active loop.

Define ⟨**variable** ⟩ ⟨**value** ⟩ Defines a numeric variable that can be used like a loop variable.

AddTo ⟨**variable**⟩ ⟨**value** ⟩ Adds a number to a previously defined variable.

Undefine ⟨**variable**⟩ Forgets the previously defined variable.

File format for single magnetization states

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The file format must contain all information necessary to reconstruct the LEM state. This includes the full mesh, and the correct length scale to define particle geometry and size. Further requirements are all Material constants A,$K1$,Ms as well as anisotropy tensor and the field direction and strength. In case of magnetostriction additional material constants include E,v,λijk.

It might be useful to represent the mesh by its MD5 hash to have a unique identifier.

Energy considerations

Energy minimization is limited by physical, numerical and algorithmic constraints.

Numerical constraints The different minimization algorithms have a limited precision. Minimization below this precision can lead to unwanted repetitions due to numerical noise. This can be related to the conjugate gradient method for the sparse matrices or to limited precision in internal functions, e.g. trigonometric functions used for transforming polar to cartesian coordinates.

Algorithmic constraints The finite mesh size or finite distances introduce grid errors and artifacts. The weak FEM solutions are elements of a finite dimensional space approximating a real physical solution. Minimizing below the corresponding approximation error is physically meaningless, even if mathemat- ically correct.

Physical constraints The micromagnetic model only represents a part of the physically relevant energies. Some energy terms are neglected, like magnetostriction, elastic, and electric energies. Most notably thermal activation is disregarded. Minimization of the energy to higher precision than the real vari- ability of the energy is physically irrelevant.

Sometimes it may be mathematically useful to perform higher precision minimizations. This could be necessary to find a complex minimization route that finally leads to a also physically better minimum.

To benchmark different algorithms it also can be useful to compare their output to unphysical degrees of precision.

In most cases it is useful to have a constantly updated estimate of the different accuracy requests to avoid unnecessary minimization steps. The thermal energy per degree of freedom is $1/2kT$. In the FEM model the number of degrees of freedom (DOF) is $2 \times NNODE$ where $NNODE$ is the number of nodes in the

mesh, because each unit vector has two DOF. The total variability in energy density ΔE is then

$$\Delta E = \frac{kT\ NNODE}{V_{tot}}$$

The mesh related discretisation error can be estimated by comparing results on two separate meshes with similar number of nodes.

To test wether a minimum is really achieved one can monitor largest angular variation along the minimization route. Close to a supposed minimum one can perturb the current state $m0$ into a state $m1$ which is a distance d away from $m0$. If after k minimization steps the result $m2$ is within $//m2 — m0// < d/k$ then $m0$ is assumed to represent an LEM.

Fluctuation field

Van de Wiele et al. (2010) state an expression for the fluctuation field in a micromagnetic model where the amplitude of the thermal fluctuations is derived from the fluctuation-dissipation theorem. A corrected and adapted version of this expression for a tetrahedral subvolume is

$$H_{therm} = \sqrt{\frac{\alpha kT}{\gamma E \mu_0^2 M_S V_{tet} \delta t}}$$