FACULTY OF SCIENCES

DEPARTMENT OF SOLID STATE SCIENCES
DYNAMAT GROUP

MUMAX3-WORKSHOP

SESSION 1

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IEEE MAGNETICS

NVIDIA

ICS INTRONICS

THE DYNAMAT TEAM

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WORKSHOP SCHEDULE

Monday 08/31, 6PM-8PM CET

Session 1: general introduction to micromagnetics in mumax3

Session 2: mumax3 ecosystem, workflow and a first simulation

Monday 09/07, 6PM-7:30PM CET

Session 3: basic examples

Homework

Monday 09/14, 6PM-7:30PM CET

Session 4: advanced features and more extensive examples

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SESSION 1: GENERAL INTRODUCTION

Part 1: Micromagnetics recap

- Magnetization field
- Magnetic energy
- Magnetization dynamics
- Energy minimization

Part 2: Design of mumax3

- Mumax3 in a nutshell
- Scripting language
- Discretization
- Shapes, geometry, regions
- Material parameters
- Initial magnetization
- Output
- Run/Relax/Minimize
- Effective field terms
- Spin transfer torques

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MICROMAGNETISM

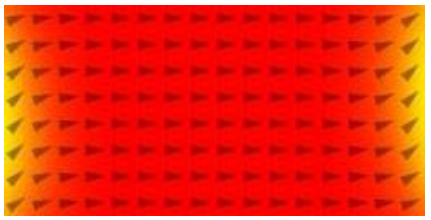
In ferromagnets, neighboring magnetic moments have the tendency to align

Continuum approx.

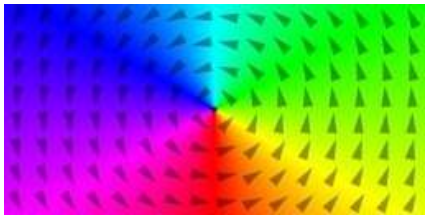
Magnetization can be described by a continuous vector field

$$\boldsymbol{M}(\boldsymbol{r},t) = M_s(\boldsymbol{r})\,\underbrace{\boldsymbol{m}(\boldsymbol{r},t)}_{\text{central quantity of interest}}$$

- picosecond time scale
- 1nm – 1µm length scale



Quasi-uniform state



Vortex

Néel Skyrmion

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MICROMAGNETISM

The physics is fully described by the total magnetic energy functional:

$$E[\boldsymbol{m}] = \int_V \Big\{ \underbrace{A(\nabla \boldsymbol{m})^2}_{\textit{Exchange}} \underbrace{- \mu_0 \boldsymbol{M} \cdot \boldsymbol{H}_{ext}}_{\textit{Zeeman}} - \frac{\mu_0}{2} \boldsymbol{M} \cdot \boldsymbol{H}_{demag} + \textit{Crystal anisotropy} \\ \textit{Dzyaloshinskii-Moriya} \\ \textit{Magneto-elasticity} \\ \textit{Higher-order exchange} \\ \ldots \Big\} d^3\boldsymbol{r}$$

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MICROMAGNETISM

Two main objectives

Time integration

dynamics

- Spin waves
- Domain wall motion
- Spin transfer torques
- Vortex excitation
- ….

Energy minimization

statics

- Stable magnetic states
- Hysteresis curves
- Phase diagrams
- Domain wall profiles
- …

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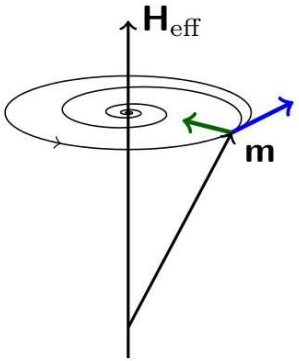
MICROMAGNETISM

Time integration
dynamics

The magnetization dynamics is described by the Landau-Lifshitz-Gilbert (LLG) equation

$$\dot{\boldsymbol{m}} = -\frac{\gamma}{1+\alpha^2}\left[\underbrace{\boldsymbol{m} \times \boldsymbol{H}_{eff}}_{\text{precession}} + \underbrace{\alpha\, \boldsymbol{m} \times (\boldsymbol{m} \times \boldsymbol{H}_{eff})}_{\text{damping}}\right] \quad \text{with} \quad \boldsymbol{H}_{eff} = -\frac{1}{\mu_0 M_s}\frac{\delta E}{\delta \boldsymbol{m}}$$



Computation of the magnetization dynamics:

$$E[\boldsymbol{m}, t] \;\rightarrow\; H_{eff}(\boldsymbol{r}) \xrightarrow{\text{LLG}} \boldsymbol{m}(\boldsymbol{r}, t)$$

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MICROMAGNETISM

Time integration
dynamics

LLG adaptation 1

Spin transfer torques (Zhang-Li[1], Slonczewski[2,3])

$$\dot{\boldsymbol{m}} = -\frac{\gamma}{1+\alpha^2}\left[\boldsymbol{m}\times\boldsymbol{H}_{eff} + \alpha\,\boldsymbol{m}\times\left(\boldsymbol{m}\times\boldsymbol{H}_{eff}\right)\right] + \tau_{STT}$$

LLG adaptation 2

Additional random effective field term which scales with the temperature[4]

$$\boldsymbol{H}_{eff} \rightarrow \boldsymbol{H}_{eff} + \boldsymbol{H}_{th}$$

$$\langle \boldsymbol{H}_{th}(\boldsymbol{r},t)\rangle = 0$$

$$\langle \boldsymbol{H}_{th}(\boldsymbol{r},t), \boldsymbol{H}_{th}(\boldsymbol{r}',t')\rangle = \frac{2k_B T\alpha}{M_s\gamma}\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t')$$

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[1] Physical Review Letters **93**(12), 127204 (2004).
[2] Journal of Magnetism and Magnetic Materials **159**(1-2), L1–L7 (1996).
[3] Physical Review B **70**(17), 172405 (2004).
[4] Journal of Applied Physics **112**(2), (2012).

MICROMAGNETISM

Energy minimization
statics

Two approaches to minimize the free energy functional numerically:

1. Standard minimization scheme (*e.g. steepest gradient*)

2. LLG equation with strong damping *(=removing the precession term)*

$$\dot{\boldsymbol{m}} = -\boldsymbol{m} \times \left(\boldsymbol{m} \times \boldsymbol{H}_{eff}\right)$$

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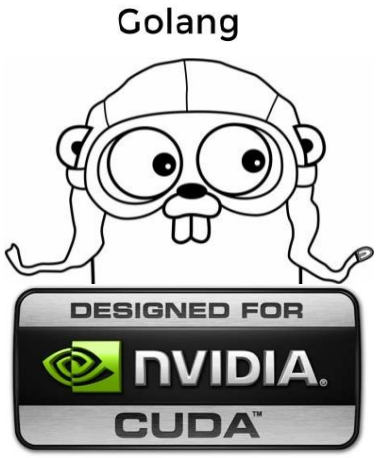
WHAT IS MUMAX3?

- Free finite-difference based micromagnetic simulation package
- GPU-accelerated *nvidia GPU required*
- Developed at DyNaMat (Ugent) by Arne Vansteenkiste
- Latest official release mumax3.10 *(Aug 13, 2020)*
- Active community *groups.google.com/forum/#!forum/mumax2*
- Documented API *mumax.github.io*
- Open source (GPLv3) *github.com/mumax/3*
- Mainly written in Go
- CUDA C kernels for heavy lifting
- Scripting language + Web GUI
- Well tested (unit tests + NIST standard problems)



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SCRIPTING LANGUAGE

Mumax3's scripting language is a subset of golang

```
// saturation magnetization
Msat = 5e6

// declare new variable
Freq := 1e9

for i:=0; i<10; i++ {
        print(i)
}

if 1+8 == 9 {
        print("Of course 1+8=9")
}
```

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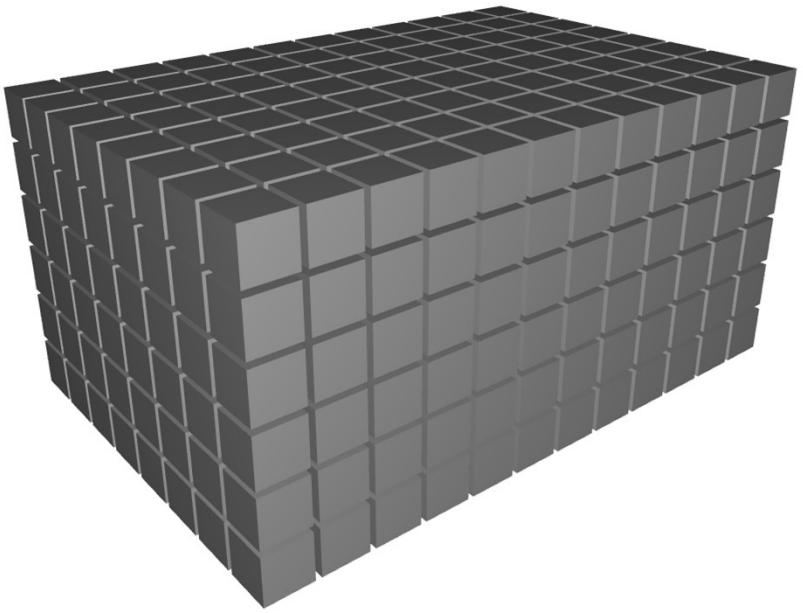
DISCRETIZATION



- Rectangular simulation box (origin in the center)
- Single regular rectangular grid
- Uniform magnetization inside cell $\boldsymbol{m}_{ijk} = \boldsymbol{m}(x_i, y_j, z_k)$
- Cell size < exchange length

```
setgridsize(256,64,1)
setcellsize(1e-9,1e-9,1e-9)
```

- PBC values are number of virtual repetitions of the simulation box used to calculate dipolar interactions

```
setpbc(4,0,0)
```

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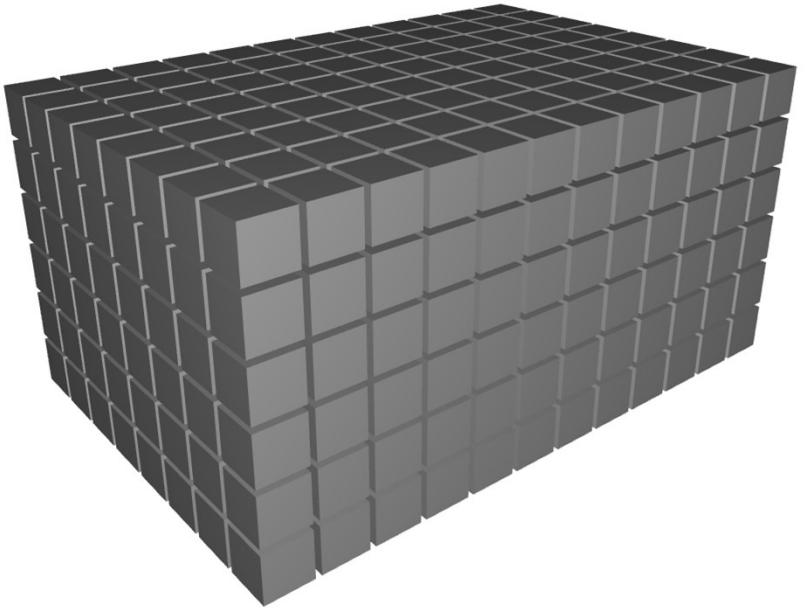
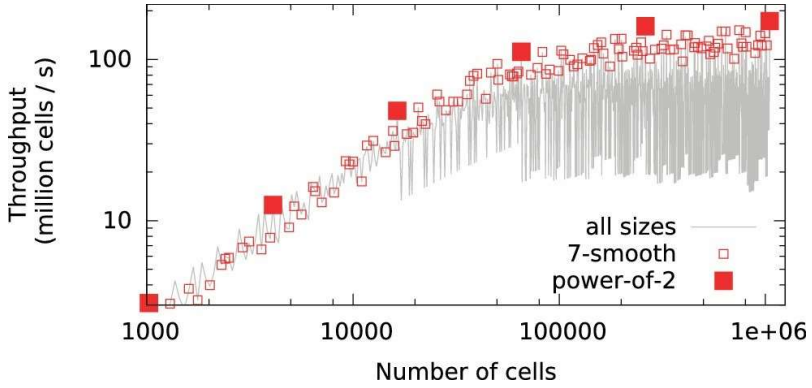
DISCRETIZATION



The cuda fft library (used for the computation of the demag field) is highly optimized for grid size dimensions with small prime factors.



Tip: try to use grid size dimensions which are '7-smooth'

Example of good and bad grid size dimensions:

$190 = 2 \cdot 5 \cdot 19$ 

$191 = 191$ 

$192 = 2^6 \cdot 3$ 

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SHAPES

- A shape can be considered as a function $f: \mathbb{R}^3 \rightarrow \{true, false\}$ where

$$f(x,y,z) = \begin{cases} true \text{ if } (x,y,z) \text{ in shape} \\ false \text{ otherwise} \end{cases}$$

- Most shapes do not depend on the grid
- Default location: center of universe (0,0,0)
- Large set of predefined basic shapes
- Define new shapes by combining and modifying the basic shapes
- Shapes are useful for different tasks:
  - The geometry
  - Defining regions
  - To set locally an initial magnetization

SHAPES

Shapes

Cell(j,k,l)
Circle(diameter)
Cone(diameter,height)
Cuboid(Lx,Ly,Lz)
Cylinder(diameter,height)
Ellipse(a,b)
Ellipsoid(a,b,c)
ImageShape(filename)
Layer(i)
Layers(i1,i2)
Rect(Lx,Ly)
Square(L)
Xrange(xmin,xmax)
Yrange(ymin,ymax)
Zrange(zmin,zmax)

Shape methods

Transl(dx,dy,dz)
Scale(sx,sy,sz)
RotX(angle)
RotY(angle)
RotZ(angle)
Repeat(dx,dy,dz)

Add(shape)
Sub(shape)
Inverse()
Intersect(shape)
Xor(shape)

```
// Rotated cheese example

d  := 200e-9
sq := square(d)

h     := 50e-9
hole  := cylinder(h, h)
hole1 := hole.transl(100e-9, 0, 0)
hole2 := hole.transl(0, -50e-9, 0)

cheese := sq.sub(hole1).sub(hole2)
cheese = cheese.rotz(pi/6)
```

rotated cheese

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GEOMETRY

Optionally a magnet Shape other than the full simulation box can be specified

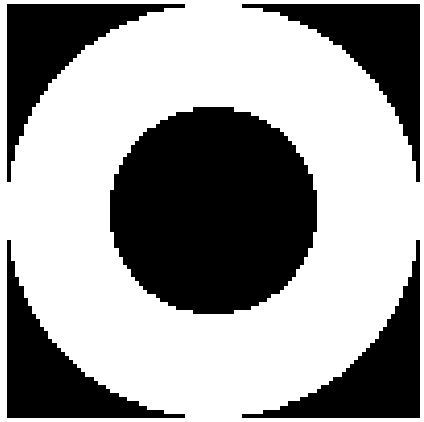
```
// Ring geometry example

setGridsize(100, 100, 10)
setCellsize(1e-9,1e-9,1e-9)

ring := circle(100e-9).sub(circle(50e-9))

setgeom(ring)

save(geom)
```



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REGIONS

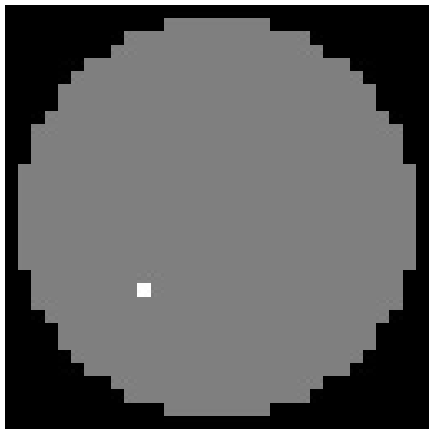
- 256 regions in total (index 0→ 255)
- Each cell is assigned to a single region (default region id is 0)
- Each region has its own set of material parameters
- Two ways to set the region id in cells:
  1. Set region id of a single cell
  2. Set region id of all cells in a shape

```
SetGridSize(32,32,1)
SetCellSize(1,1,1)

// Set region id of cells in a circle to 1
DefRegion(1, circle(30))

// Set region id of cell (10,10,0) to 2
DefRegionCell(2, 10, 10, 0)

Save(regions)
```



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MATERIAL PARAMETERS

- Material parameters are assigned to the 256 regions.
- Material parameters can be functions of time
- There are vector and scalar material parameters
- Material parameters are predefined, they can not be created

```
// Assigning to a material parameter sets a value in all regions:
Msat  = 800e3
AnisU = vector(1, 0, 0)

// When regions are defined, they can also be set region-wise:
Msat.SetRegion(0, 800e3)
Msat.SetRegion(1, 540e3)

// Material parameters can be functions of time as well:
f := 500e6
Ku1 = 500 * sin(2*pi*f*t)
```

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MATERIAL PARAMETERS: EXCITATIONS

- An excitation is a regional material parameter
- Additionally, one can add an arbitrary number of time- and space-dependent vector fields of the form :

$$g(x_i, y_j, z_k) * f(t)$$

```
B_ext = vector(0,0,1)

B_ext.Add(LoadFile("antenna.ovf"), sin(2*pi*f*t))

B_ext.removeExtraTerms()
```

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INITIAL MAGNETIZATION

Different ways to set the magnetization:

```
m = config
m.LoadFile(filename)
m.SetRegion(regionId, config)
m.SetInShape(shape, config)
m.SetCell(j,k,l, vector)
```

Here, a ‘config’ is an object which represents a magnetization configuration

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INITIAL MAGNETIZATION

Config

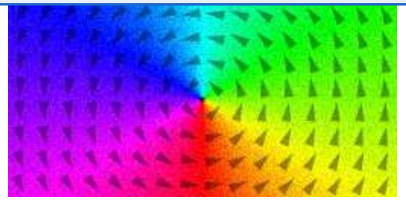
Uniform(mx, my, mz)
RandomMag()
RandomMagSeed(seed)
TwoDomain(
  mx1, my1, mz1,
  my2, my2, mz2,
  mx3, my3, mz3)
Vortex(circ, pol)
AntiVortex(circ, pol)
VortexWall(mxLeft, mxRight, circ, pol)
NeelSkyrmion(charge, pol)
BlochSkyrmion(charge, pol)
Conical(kVec, coneDir, coneAngle)
Helical(kVec)

Config methods

Transl(dx,dy,dz)
Scale(sx,sy,sz)
Add(ratio, config)
RotZ(angle)

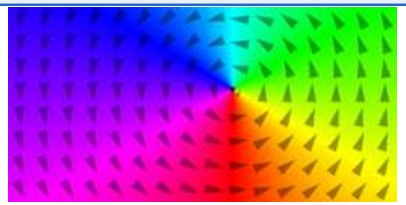
```
m = uniform(1,1,0)
```

```
m=Vortex(1,-1).Add(0.1,randomMag())
```

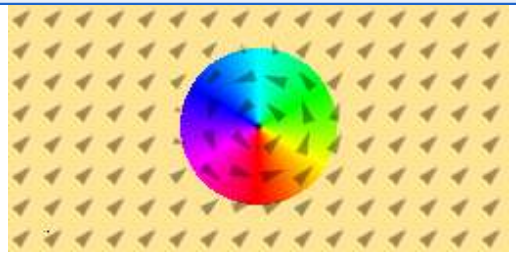


```
M = BlochSkyrmion(1, 1)
```

```
m=Vortex(1,-1).transl(100e-9,50e-9,0)
```



```
m = uniform(1, 1, 1)
m.setInShape(cylinder(400e-9,100e-9), vortex(1,-1))
```



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OUTPUT

3 output media:

- log file for input, logging and printing
- table.txt (t, mx, my, mz, …)

```
tableadd(E_total)
tableaddvar(myVar,”myVar”,”unit”)
tablesave() // write single line
tableautosave(1e-12) // write periodically
```

- .ovf files for scalar and vector fields

```
save(Edens_total)
saveas(Edens_total,”edens.ovf”)
autosave(Edens_total, 1e-10) // write perdiodically
```

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RUN/RELAX/MINIMIZE

- Solving the LLG equation (time integration)

```
run(timeperiod)
steps(100)
runWhile(condition)
```

- Minimizing the energy

```
relax()    // LLG without precession
Minimize() // steepest descent[1]
```

```
// WARNING: ADVANCED SETTINGS
// In most cases, these settings can be ignored

// Set the solver:
//   1:Euler, 2:Heun, 3:Bogaki-Shampine, 4: Runge-Kutta(RK45),
//   5:Dormand-Prince(the default), 6:Fehlberg, -1:Backward Euler
SetSolver(5)

// set timestep
fixdt = 0 // if 0 (default): use adaptive timestep

// Advanced settings for adaptive timestep (default values are given)
Headroom = 0.8 // headroom dt correction
MaxDt = 0      // if 0, no maximal timestep
MinDt = 0      // if 0, no minimal timestep
MaxErr = 1e-5  // maximum allowed error/step

// Advanced settings for minimizer (default values are given)
MinimizerSamples = 10 //Number of max dM for convergence check
MinimizerStop = 1e-6  //Stopping max dM for Minimize
```

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[1] JOURNAL OF APPLIED PHYSICS115, 17D118 (2014)

THE INTERACTIONS

Effective field terms

- Demagnetization
- Exchange
- Anisotropy
- Dzyaloshinskii-Moriya
- External field
- Thermal field
- Custom field

Spin transfer torques

- Zhang-Li STT
- Slonczewski STT

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DEMAGNETIZATION FIELD TERM

Demagnetization energy density

$$\varepsilon = -\frac{\mu_0}{2} M_s \boldsymbol{m} \cdot \boldsymbol{H}_{demag}$$

Regional Material Parameters	
`Msat`	Saturation magnetization (A/m)
`NoDemagSpins`	Disable magnetostatic interaction per region (default=0, set to 1 to disable).

Output Quantities	
`B_demag`	Magnetostatic field (T)
`Edens_demag`	Magnetostatic energy density (J/m3)
`E_demag`	Magnetostatic energy (J)

Other functionalities	
`EnableDemag`	Enables/disables demag (default=true)
`SetPBC`	Sets the number of repetitions in X,Y,Z to create periodic boundary conditions. The number of repetitions determines the cutoff range for the demagnetization.
`DemagAccuracy`	Controls accuracy of demag kernel

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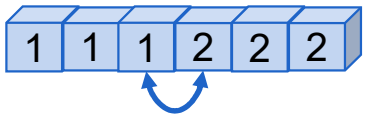
EXCHANGE FIELD TERM

Exchange energy density

$$\varepsilon = \mathrm{A}\,(\nabla \boldsymbol{m})^2$$

Harmonic mean for inter-region exchange coupling (default behavior)

$$\frac{A}{M_s} = 2\,\frac{\frac{A_1}{M_{s_1}}\frac{A_2}{M_{s_2}}}{\frac{A_1}{M_{s_1}} + \frac{A_2}{M_{s_2}}}$$



Regional Material Parameters	
`Aex`	Exchange stiffness (J/m)
`Msat`	Saturation magnetization (A/m)

Output Quantities	
`B_exch`	Exchange field (T)
`Edens_exch`	Total exchange energy density (including DMI) (J/m3)
`E_exch`	Total exchange energy (including DMI) (J)
`MaxAngle`	Maximum angle between exchanged coupled spins (rad)

Other functionalities	
`Ext_InterExchange`	Sets exchange coupling between two regions
`Ext_ScaleExchange`	Re-scales exchange coupling between two regions

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ANISOTROPY FIELD TERM

Uniaxial anisotropy energy density

$$\varepsilon = -K_1 (\hat{u} \cdot \boldsymbol{m})^2 - K_2 (\hat{u} \cdot \boldsymbol{m})^4$$

Similar expression for cubic anisotropy energy density [1]

Regional Material Parameters	
`anisU`	Uniaxial anisotropy direction
`Ku1, Ku2`	Uniaxial anisotropy constants (J/m3)
`AnisC1, AnisC2`	Cubic anisotropy directions
`Kc1, Kc2, Kc3`	Cubic anisotropy constants (J/m3)
`Msat`	Saturation magnetization (A/m)

Output Quantities	
`B_anis`	Anisotropy field (T)
`Edens_anis`	Total anisotropy energy density (including DMI) (J/m3)
`E_anis`	Total anisotropy energy (including DMI) (J)

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[1] "The design and verification of mumax3", AIP Advances 4, 107133 (2014).

DZYALOSHINSKII-MORIYA FIELD TERM

Interfacially-induced DMI energy density

$$\varepsilon = D\,[m_z(\nabla \cdot \boldsymbol{m}) - (\boldsymbol{m} \cdot \nabla)m_z]$$

Bulk DMI energy density

$$\varepsilon = D\,\boldsymbol{m} \cdot (\nabla \times \boldsymbol{m})$$

Note:

Only single DMI type allowed at once

Regional Material Parameters	
`Dind`	Interfacially-induced DMI strength (J/m2)
`Dbulk`	Bulk DMI strength (J/m2)
`Msat`	Saturation magnetization (A/m)

Output Quantities	
`B_exch`	Exchange field (including DMI) (T)
`Edens_exch`	Total exchange energy density (including DMI) (J/m3)
`E_exch`	Total exchange energy (including DMI) (J)

Other functionalities	
`Ext_InterDind`	Sets Dind coupling between two regions
`Ext_ScaleDind`	Re-scales Dind coupling between two regions
`OpenBC`	Use open boundary conditions (default=false, use Neumann BC). This setting is only relevant for DMI.

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EXTERNAL FIELD TERM

Zeeman energy density

$$\varepsilon = -M_s \boldsymbol{m} \cdot \boldsymbol{B}_{ext}$$

Regional Material Parameters	
`Msat`	Saturation magnetization (A/m)
Excitation	
`B_ext`	Externally applied field(T)

Output Quantities	
`B_ext`	Externally applied field(T)
`Edens_zeeman`	Zeeman energy density (J/m3)
`E_zeeman`	Zeeman energy (J)

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THERMAL FIELD TERM

$$\langle \boldsymbol{H}_{th}(\boldsymbol{r},t)\rangle = 0$$

$$\langle \boldsymbol{H}_{th}(\boldsymbol{r},t), \boldsymbol{H}_{th}(\boldsymbol{r}',t')\rangle = \frac{2k_B T\alpha}{M_s\gamma}\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t')$$

Regional Material Parameters	
`Temp`	Temperature (K)
`alpha`	Damping parameter
`Msat`	Saturation magnetization (A/m)

Output Quantities	
`B_therm`	Thermal field (T)
`Edens_therm`	Thermal energy density (J/m3)
`E_therm`	Thermal energy (J)

Other functionalities	
`ThermSeed`	Sets random seed for thermal noise

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CUSTOM FIELD TERMS

Output Quantities	
`B_custom`	User-defined field (T)
`Edens_custom`	Total energy density of user-defined field (J/m3)
`E_custom`	Total energy of user-defined field (J)

Other functionalities	
`AddEdensTerm`	Add a custom energy density term
`AddFieldTerm`	Add a custom effective field term
`RemoveCustomFields`	Remove all custom fields

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ZHANG-LI STT

Zhang-Li spin-transfer torque

$$\boldsymbol{\tau} = \frac{1+\xi\alpha}{1+\alpha^2}\boldsymbol{m}\times(\boldsymbol{m}\times(\boldsymbol{u}\cdot\nabla)\mathbf{m}) + \frac{\xi-\alpha}{1+\alpha^2}\boldsymbol{m}\times(\boldsymbol{u}\cdot\nabla)\boldsymbol{m}$$

with

$$\boldsymbol{u} = \frac{\mu_B P}{2e\gamma_0 M_s(1+\xi^2)}\boldsymbol{j}$$

Regional Material Parameters	
`Pol`	Electrical current polarization
`xi`	Non-adiabaticity of spin-transfer-torque
`alpha`	Damping parameter
`Msat`	Saturation magnetization (A/m)
Excitation	
`J`	Electrical current density (A/m2)

Output Quantities	
`STTorque`	Spin-transfer torque/γ0 (T)

Other functionalities	
`DisableZhangLiTorque`	Disable Zhang-Li torque (default=false)

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SLONCZEWSKI STT

Slonczewski spin-transfer torque

$$\boldsymbol{\tau} = \beta \frac{\epsilon + \alpha\epsilon'}{1+\alpha^2} \boldsymbol{m} \times (\boldsymbol{m}_P \times \mathbf{m}) - \beta \frac{\epsilon' - \alpha\epsilon}{1+\alpha^2} \boldsymbol{m} \times \boldsymbol{m}_P$$

with

$$\beta = \frac{j_z \hbar}{M_s e\, d}$$

$$\epsilon = \frac{P\Lambda^2}{(\Lambda^2+1) + (\Lambda^2-1)(\boldsymbol{m} \cdot \boldsymbol{m}_P)}$$

Regional Material Parameters	
`Pol`	Electrical current polarization
`Lambda`	Slonczewski Λ parameter
`EpsilonPrime`	Slonczewski secondairy STT term ε'
`alpha`	Damping parameter
`Msat`	Saturation magnetization (A/m)
`FreeLayerThickness`	Slonczewski free layer thickness (if set to zero (default), then the thickness will be deduced from the mesh size) (m)
Excitation	
`J`	Electrical current density (A/m2)
`FixedLayer`	Slonczewski fixed layer polarization

Output Quantities	
`STTorque`	Spin-transfer torque/γ0 (T)

Other functionalities	
`DisableSlonczewskiTorque`	Disables Slonczewski torque (default=false)
`FixedLayerPosition`	Position of the fixed layer: FIXEDLAYER_TOP, FIXEDLAYER_BOTTOM (default=FIXEDLAYER_TOP)

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