MIFCraft for OOMMF Users

v0.3 - Mark Mascaro (doublemark@mit.edu)

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1 Introduction

MIFCraft is a Python-based scripting system designed to make writing MIF files easier and more reliable. It wraps the OOMMF-extended Tcl system entirely, and presents a pure-Python interface used to generate files. It provides simple, plain-English warnings if you typo a label, include a non-existent file, or do something else that would generate a verbose OOMMF runtime error later on. Once you're comfortable with the system, you can (for example) use simple Python looping constructs to rapidly generate groups of simulations that vary one or more parameters. To use MIFCraft, you'll need to install Python from python.org.

For this manual, it's assumed that you know OOMMF, but have never used Python. Don't worry if you don't know Python; the system is very straightforward and a few examples will go a long way. If you have used Python before, bear with me. MIFCraft has been tested with Python 2.6 and 2.7, but should be compatible with 3.0. You'll need to copy MIFCraft.py into a Python library folder, or make sure it's in the same directory as your MIFCraft scripts. This folder is most likely C:\Python26\Lib\site-packages\ for Python 2.6, C:\Python27\Lib\site-packages\ for Python 2.7, etc.

2 Getting Started with a Simple Example

Let's start with a very simple task: defining a rectangular prism of magnetic material and relaxing it from a random initial state. The final result of this is available as test.py in the SimpleExample folder where you unpacked MIFCraft. Follow along by creating your own file, first_try.py.

2.1 Some Boilerplate

All MIFCraft scripts start by importing the MIF object from the MIFCraft library. When you create a MIF object, MIFCraft creates a MIF file for OOMMF.

```
from mifcraft import MIF
```

In this example, we're also going to use the mks value of μ_0 . We define that constant based on pi, which is available in the Python math library. Later, we'll use this in our script - no need for [subst] or [expr] as normally seen in MIF files.

```
from math import pi
Mu0 = pi * 4e-7
```

Now we're ready to create our MIF object and file. We're going to use the filename test_1.mif, with the OOMMF basename test_1. As a reminder, the basename is the prefix applied to OOMMF output files. Whenever you want to supply a string of text in MIFCraft, surround it with single quotes.

```
with MIF(filename='test_1.mif', basename='test_1') as myMIF:
```

We now have a MIF object named myMIF and can create Specify blocks in it. If you're reading along in the example file, you'll note that every line after this is indented. Unlike Tcl, Python cares about indentation: these indents signify that these lines belong to the the MIF file we opened with with. When you stop indenting, that's a sign that you're done setting up this MIF file and want it written out.

One last aside: whenever you'd like to provide extra clarity, you can put comments in your MIFCraft files using the # character. This causes the rest of the line to be ignored.

2.2 Replacing Specify...

In a normal MIF file, you'd probably start with some geometry, something like:

```
Specify Oxs_BoxAtlas:SomeAtlas {
    xrange { 0   1e-7 }
    yrange { 0   1e-7 }
    zrange { 0   2e-8 }
}
```

In MIFCraft, we create this in myMIF like this:

```
myMIF.BoxAtlas(xrange=(0, 100e-9),
yrange=(0, 100e-9),
zrange=(0, 20e-9))
```

For each Specify... statement you can use in OOMMF, there's a corresponding method in MIFCraft with the same name, minus 'Oxs_'. Each parameter that needs to be specified in OOMMF as 'name value' is specified here as 'name=value'. Note how the ranges are grouped with parentheses. A complete manual on how to specify parameters for each type of Specify block is provided in mifcraft-reference.html, but you'll find most of them are obvious.

You'll note this atlas doesn't have a name (like 'SomeAtlas'). That name is automatically generated by MIFCraft, and you don't have to worry about it. What if we want to use this atlas later on? Well, we can capture it like this:

This is what's done in the example file. Now we can reference that atlas by its Python name, 'Brick'. We do this immediately when we create the mesh:

Remember to indent, and once again, group multiple values with parentheses. Note that Brick isn't a string and doesn't need single quotes-it's a Python name, like myMIF.

We also need our standard parameters: demagnetization and exchange energy.

```
myMIF.Demag()
myMIF.UniformExchange(A=13e-12)
```

Next we need an evolver - we'll use Oxs_RungeKuttaEvolve. Most parameters have default values here, so we only need one. Let's do a quasistatic simulation.

```
myMIF.RungeKuttaEvole(alpha=0.5)
```

We'd like to move on to our Oxs_TimeDriver, but we know that takes a scalar field for saturation magnetization and a vector field for initial magnetization. We set those up first and assign them labels, then use them directly.

Note that we didn't give the TimeDriver an Evolver, which it needs. MIFCraft knows you'll only ever create one Evolver per MIF file, and links the TimeDriver to it automatically! All we have left to do is set up outputs.

All told, your file should now look like this:

```
from mifcraft import MIF
from math import pi
Mu0 = pi * 4e-7
with MIF(filename='test_1.mif', basename='test_1') as myMIF:
    Brick = myMIF.BoxAtlas(xrange=(0, 100e-9),
                            yrange = (0, 100e - 9),
                            zrange=(0, 20e-9))
    myMIF.RectangularMesh (atlas=Brick,
                           cellsize = (5e-9, 5e-9, 5e-9)
    myMIF.Demag()
    myMIF. UniformExchange (A=13e-12)
    myMIF.RungeKuttaEvole(alpha=0.5)
    myMs = myMIF.UniformScalarField(value=800e3)
    mym0 = myMIF.PlaneRandomVectorField(min_norm=1,
                                          max_norm=1,
                                          plane_normal = (0, 0, 1))
    myMIF. TimeDriver(stopping_dm_dt = 0.1,
                      stage_count=1,
                      Ms = myMs,
                      m0 = mym0)
```

Now we can run that file with python first_try.py from the command line, or by opening and then running it in the IDLE editor that comes with your Python installation, if you'd rather. I like the command line. (You can also run .py files directly from the Windows Explorer shell, but you won't be able to see the debug information if you have any mistakes!) That will create test_1.mif in the same folder, and it looks like this:

```
# MIF 2.1
# Auto-generated by MIFCraft at 15:19:56 on Tuesday Jan 10 2012
Specify Oxs_BoxAtlas:BoxAtlas {
    xrange { 0.00e+00 1.00e-07 }
    yrange { 0.00e+00 1.00e-07 }
    zrange { 0.00e+00 \ 2.00e-08 }
}
Specify Oxs_RectangularMesh:RectangularMesh {
    cellsize { 5e-09 5e-09 5e-09 }
    atlas BoxAtlas
}
Specify Oxs_Demag:Demag {}
Specify Oxs_UniformExchange:UniformExchange {
    A 1.3e-11
Specify Oxs_RungeKuttaEvolve:RungeKuttaEvolve {
    alpha 0.5
    do_precess 1
    allow_signed_gamma 0
Specify Oxs_UniformScalarField:UniformScalarField {
    value 800000.0
{\tt Specify \ Oxs\_PlaneRandomVectorField:PlaneRandomVectorField \ \{ \ \ \ \} \ }
    plane_normal { 0 0 1 }
    min_norm 1
    max_norm 1
Specify Oxs_TimeDriver:TimeDriver {
    evolver RungeKuttaEvolve
    mesh RectangularMesh
    Ms UniformScalarField
    mO PlaneRandomVectorField
    \tt basename test\_1
    stage_count 1
```

```
stopping_dm_dt 0.1
}

Destination disp mmDisp
Schedule Oxs_TimeDriver:TimeDriver:Magnetization disp Step 50
```

2.3 Debugging with MIFCraft

divide atlas y size 1e-07

That's nice, and it produces a pretty and well-formatted MIF file, but it didn't save us that much work! We still wrote everything by hand. To see one aspect where MIFCraft comes in handy in this example, let's deliberately introduce an error in our Python file - let's change the cell size so that it doesn't divide cleanly.

```
myMIF.RectangularMesh(atlas=Brick,
cellsize=(5e-9, 6e-9, 5e-9))
```

When we try to run this, we get the following error:

```
(.\test_1.mif) could not be completed:
In RectangularMesh <RectangularMesh>: ystep invalid: 6e-09 does not evenly
```

We're given the exact location and nature of the error before we even try loading the file in OOMMF. If we make the same mistake in a MIF file, we instead see:

```
Error loading test_1.mif: Error thrown from inside "Oxs_ExtCreateAndRegister" --- Oxs_Ext initialization error
in construction of Oxs_RectangularMesh:RectangularMesh --- Oxs_Ext ERROR: Invalid MIF input block detected
for object Oxs_RectangularMesh: RectangularMesh: range is not an integral multiple of cellsize.
(LoadProblem)
Message time: Wed Jan 11 3:33:10 PM Eastern Standard Time 2012
Message id: crc: 0x0FDE56B5 413
Message src: Oxs_Mif
STACK TRACE:
Error loading test_1.mif: Error thrown from inside "Oxs_ExtCreateAndRegister" --- Oxs_Ext initialization error
in construction of Oxs_RectangularMesh:RectangularMesh --- Oxs_Ext ERROR: Invalid MIF input block detected
for object Oxs_RectangularMesh: RectangularMesh: range is not an integral multiple of cellsize.
while executing
"Oxs_ExtCreateAndRegister $key $init_str" ('Oxs_Mif' instance method 'ReadMif' line 108)
invoked from within
"_Oxs_Mif1 ReadMif {test_1.mif} {}"
invoked from within
"Oxs_ProbInit $f $MIF_params"
```

That is a stack trace, and it's a very useful error message for programmers, but not quite what you want when you're just working on a MIF file. Let's try another error - just delete the yrange part of our BoxAtlas.

```
(.\test_1.mif) could not be completed:
  In BoxAtlas <BoxAtlas>: yrange invalid: mandatory argument 'yrange' not
  provided.
```

If a response has to be one of a fixed list, you'll be informed of what the valid options are. If we change the type of our Destination to 'mmLies', we get:

```
(.\test_1.mif) could not be completed:
   In Destination mmLies <disp>: type invalid: mmLies is not one of ['mmDisp',
'mmGraph', 'mmArchive', 'mmDataTable'].
```

You'll also be warned if you create any Specify blocks that you never use (typically unused atlases), if you reference any files that don't exist (such as images), or if you don't set up any output for your simulation. You might have intended this for some reason, so your file will still be created - it's just a warning.

2.4 Using Names Manually

Sometimes, usually when you want to schedule some kind of output, you may want to supply a name instead of using the hidden MIFCraft auto-names. You can do this by adding the extra argument 'name' to anything.

In most cases, names will be obvious - the Oxs_TimeDriver is called TimeDriver, the Oxs_UZeeman is called UZeeman, and so on. If you have more than one of a particular energy, though, you may find it helpful to use manual names to set up your output.

3 Using Python: A More Advanced Example

Now we can apply control flow concepts that are missing from MIF files, partcularly for loops. We're also going to make some use of Python lists and string substitution.

3.1 Python Lists in Five Seconds

A list is surrounded by square brackets []. It can contain any number of items. For example, [1, 2, 3, 4, 5] is a list of numbers. You can make an empty list with []. To add something to a list, use nameOfList.append(something). For example,

```
foo = [1, 2, 3]
foo.append(5)
```

foo is now the list [1, 2, 3, 5].

In MIFCraft, lists of names of Specify blocks are often handy in creating MultiAtlases.

3.2 Python For Loops in Five Seconds

A for loop repeats a block of code several times, changing the value of a variable each time.

```
for foo in ["a", "b", "c"]:
    print foo
```

prints a, then b, then c. We can use this to create multiple MIF files, varying one or more parameters.

3.3 Python String Substitution in Ten Seconds

You can use '%s' in a string to copy the value of a variable into that string. The string is followed by % and then the variable names. For example,

```
foo = 'inserted'
print 'You'll see the variable %s here.' % (foo)
   prints 'You'll see the variable inserted here.' You can use multiple variables like this:
foo = 'see'
bar = 'inserted'
print 'You'll %s the variable %s here.' % (foo, bar)
```

3.4 Python Ranges in Five Seconds

When creating loops, you'll often want to create a range of evenly spaced numbers for parameter variation. Here you should use the command range(min, max, step), which gives all numbers between min (inclusive) and max (exclusive) separated by the given step. If no step is given, it's assumed to be 1. For example, range(1, 6, 2) gives [1, 3, 5]. Remember the exclusivity: range(1, 5, 2) gives [1, 3]. So, instead of

3.5 Varying Parameters in MIF Files

Let's assume that for some reason we really want to do the same simulation as in our first example, only we really want to try the simulation at various values for the saturation magnetization, say 500e3 to 1100e3. We don't want every single one, so let's do 500e3, 600e3, 700e3, and so on. Let's modify our script to produce several different MIF files, each the same except for the saturation magnetization. We'll want to make a MIF file for each one. For convenience, let's put them all in a subdirectory mifs. We can do this very easily:

This will create seven output files in the mifs subdirectory, named sat_500e3.mif, sat_600e3.mif, and so on. The same technique can be used to vary any parameter you like. If you want to explore a two-dimensional parameter space, you can do something like

```
for firstParam in range(1, 10, 1):
    for secondParam in range(50, 250, 50):
        with MIF(...)
...
```

and all possible pairs will be used. All you need to do is choose appropriate filenames and basenames.

In the HideousExample subfolder, there is an example from my recent research: a permalloy bar with conductive gold pads attached to it at regular intervals. This causes the current density through the bar and the Oersted field generated by the pads to modulate along its length of the bar. Additionally, the geometry of the gold pads can be varied to modulate the current drop vs. the resultant Oersted field... and the pads can be placed above or below the pad, changing the sense of the Oersted field for a propagating domain wall of given chirality. The Oersted field was previously modeled, so it's just a matter of plugging in numbers. Modulating these parameters means defining plenty of BoxAtlases in each simulation to capture all the different regions!

In this case, my MIFCraft script was just over 100 lines, including some comments. This produced 1,282 distinct simulation files, each over 700 lines long! Good thing OOMMFq can control batches of simulations. When there's some amount of symmetry in the problem, using loops with MIFCraft can save plenty of work. Take a look at a Python tutorial and see what you can do.

4 Common Tricks

4.1 Organizing MIF Files and Data

It's possible to use MIFCraft to generate really enormous volumes of data. I've found it's useful to put all my MIF files in one folder, and all the outputs in another folder with subfolders for each MIF file. For example, if I have MIFs/foo.mif and MIFs/bar.mif, the output will be in data/foo/ and data/bar. Since MIFCraft generates directories automatically as needed, this is easily accomplished as follows.

Using string substitution in folder names is an easy way to keep data well-sorted.

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