OOMMF on nanoHUB: First-Time User Guide v.2

OOMMF is the Object Oriented MicroMagnetic Framework, which is a powerful research-grade simulation tool for modeling the response of materials to applied magnetic fields that was developed by Drs. Mike Donahue, Don Porter and Robert McMichael at the National Institute of Standards and Technology (NIST). Ongoing development and maintenance are provided by Drs. Mike Donahue and Don Porter in the Information Technology Laboratory at NIST.

This first-time user guide demonstrates how to download, read and run an OOMMF example problem file in OOMMF *running on nanoHUB*, and is written for the first-time OOMMF user. No software installation or local computational power is required. If you have a computer, tablet or other device that is equipped with a **web browser** and a **connection to the Internet**, you can run OOMMF on nanoHUB. Experienced OOMMF users should find all of the functionality they are accustomed to.

In order to run simulations on nanoHUB.org, a **user account** is required. Accounts are free and simple to set up, either from links on the nanoHUB main page https://nanohub.org/ or by going directly to: https://nanohub.org/register/.

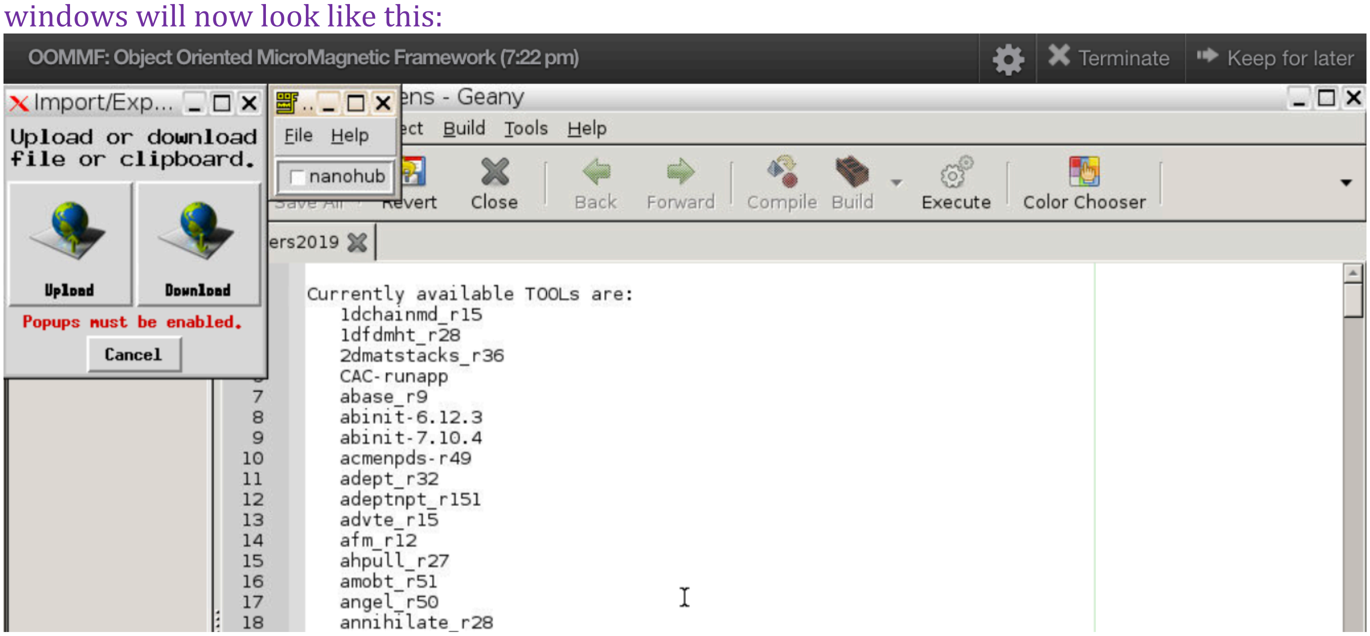
In your web browser, navigate to the OOMMF tool page: https://nanohub.org/tools/oommf/. Note that there are several tabs with information about OOMMF, including *Supporting Docs*, which includes the full OOMMF user guide, OOMMF quick start guide, and this first-time user guide.

To launch OOMMF on nanoHUB, **click on the blue "*Launch tool*" button.**

**** New in May 2020 ****

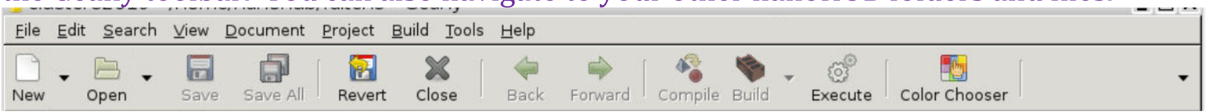
The Geany text editor has been added to the OOMMF window in nanoHUB, and is set up to recognize .mif files. The Geany manual is here: https://www.geany.org/documentation/manual/ .

The Geany window will show up full screen behind the other OOMMF windows. The initial OOMMF windows will now look like this:

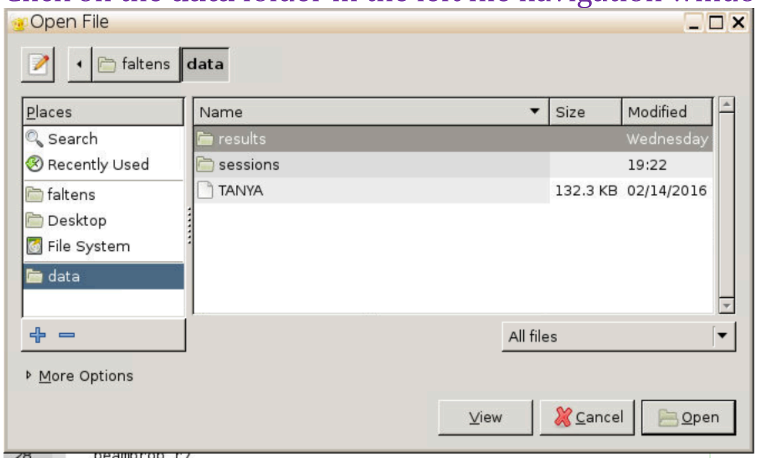


The top two windows are the same as before (when they were on a blue background, as is shown in the original sections of this FTUG.)

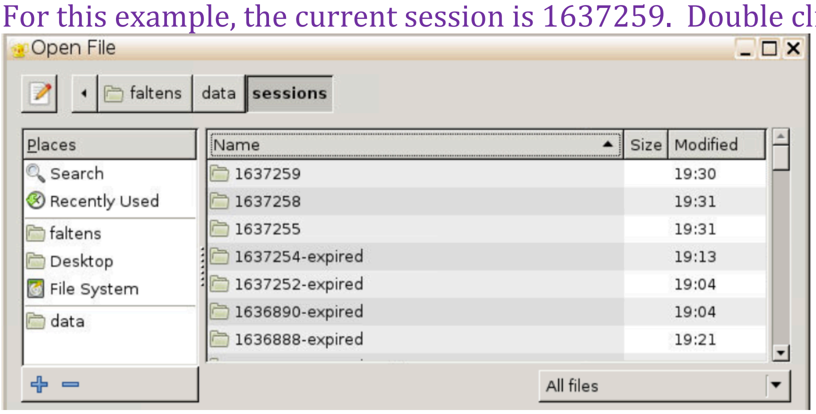
To find and edit the files in your current session, click on the Geany window, then click on "Open" in the Geany toolbar. You can also navigate to your other nanoHUB folders and files.



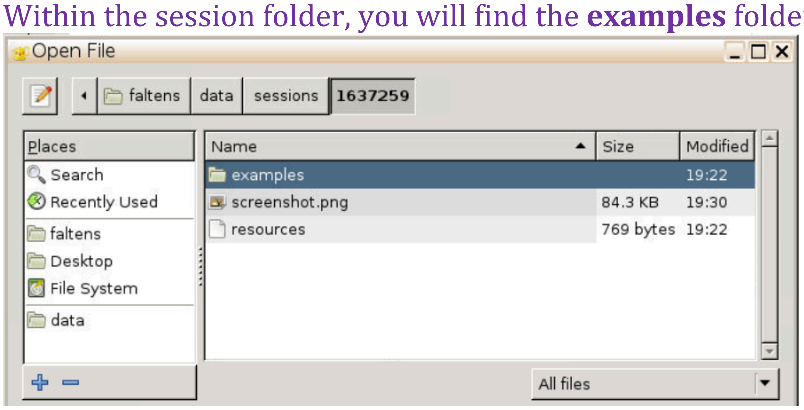
Click on the **data** folder in the left file navigation window:



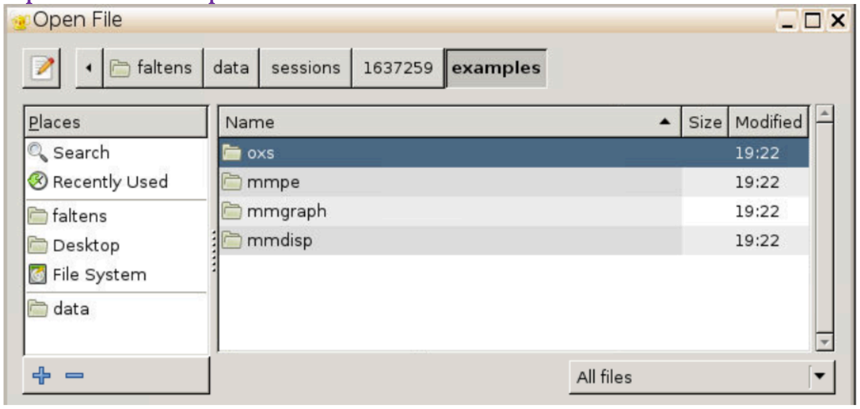
From there, double-click on **sessions**. You will see folders for your current and expired sessions. For this example, the current session is 1637259. Double click on your session folder.



Within the session folder, you will find the **examples** folder.

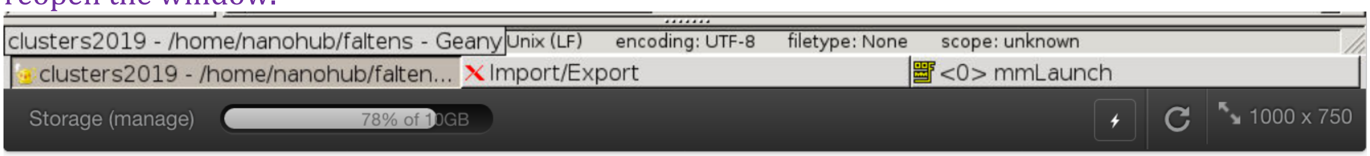


Open the examples folder:



The oxs and mmpe folders contain .mif files that you can open and edit with Geany.

You can minimize the Geany window using controls in the top right corner of the Geany window, , or by clicking on the Geany tab along the bottom of the main OOMMF window (in this example, the yellow icon with **clusters2019** - /home/...). Clicking on the Geany tab again will reopen the window.



Helpful tip: you can add the session number to the name of the session to help you keep track of your open sessions in your nanoHUB Dashboard and browser tabs. Here is an example for another session of OOMMF.

Check the URL of the browser window to see your current session number, in this case 1637255:

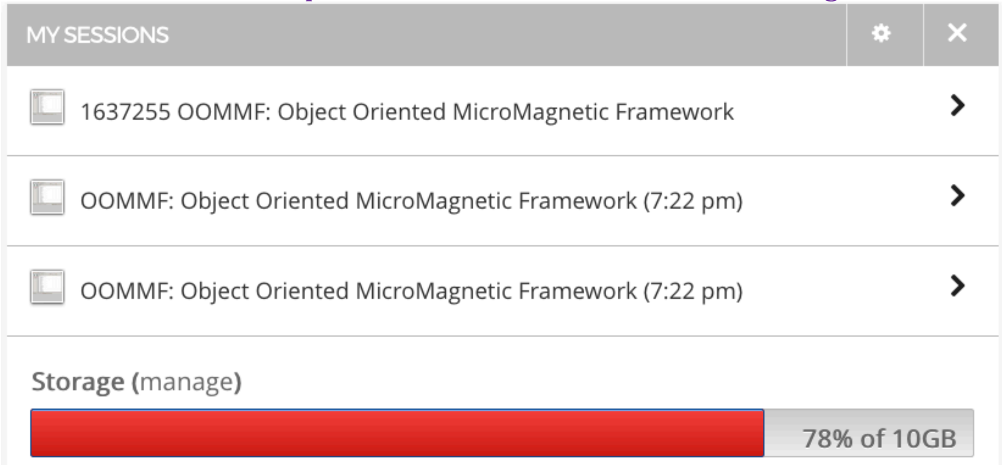
Make a note of the session number in order to find the files launched by this session of OOMMF in nanoHUB. For convenience, you can copy the session number and add it to the title of the OOMMF window. This is the way the original window title appears:

Double-click on the title OOMMF: Object Oriented MicroMagnetic Framework to open the editor:

Add the session number and click OK. Here is the updated title:

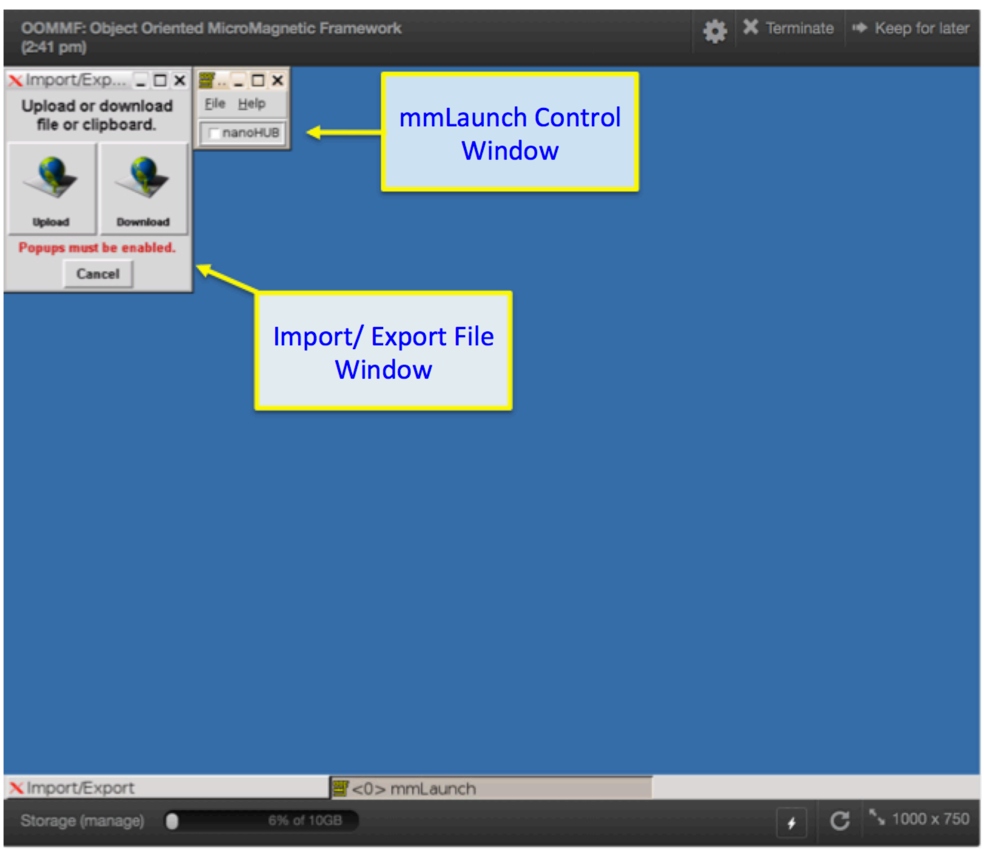
If you have more than one session running OOMMF in nanoHUB, you can now distinguish the sessions by these session numbers. You can view your active sessions in your nanoHUB Dashboard, which is available by hovering your cursor over "Logged in" in the upper right corner of a main nanoHUB window.

Here is an example of the **My Sessions** Module in the Dashboard, showing one OOMMF session whose title has been updated with the session number, along with two other unedited sessions:



*** End of new section – some other updated parts are shown in purple***

Launching OOMMF opens the main *OOMMF* window, in which two smaller windows will appear. The ***Import/Export* window** uploads and downloads files from your local computer.
The ***mmLaunch* control window** connects to the server on nanoHUB. The *mmLaunch* control window is initially very small, and may take a moment to appear.

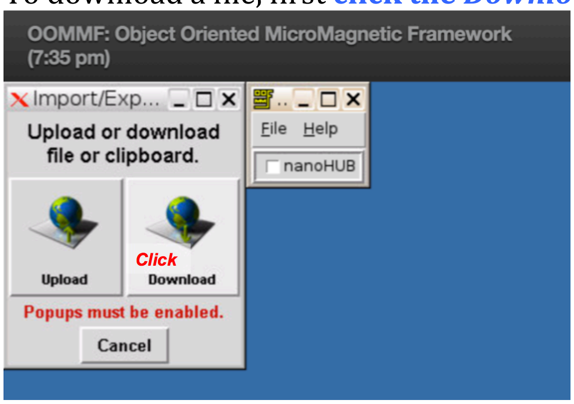


All of the windows, including the main OOMMF window, can be resized by dragging a corner. The *mmLaunch* window will automatically resize itself when it contains more items to display. If you increase the size of the *mmLaunch* control window, you will see that there is a *<0>* preceding *mmLaunch* in the window title bar. Each subsequent window that you open during the OOMMF session will be numbered incrementally. Do not worry if the numbers you see locally do not match the numbers shown in this guide, this just means the windows were opened in a different sequence.

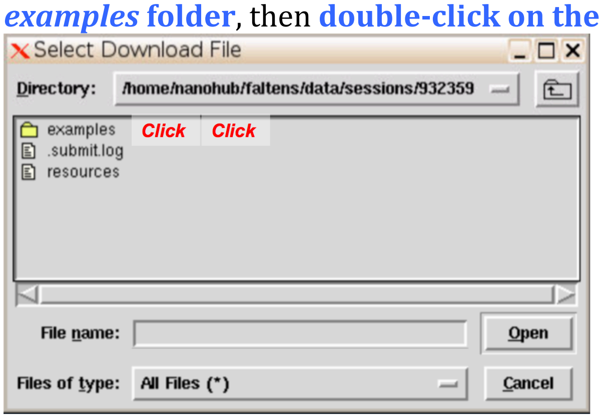
Uploading, Downloading and Viewing an OOMMF Problem File

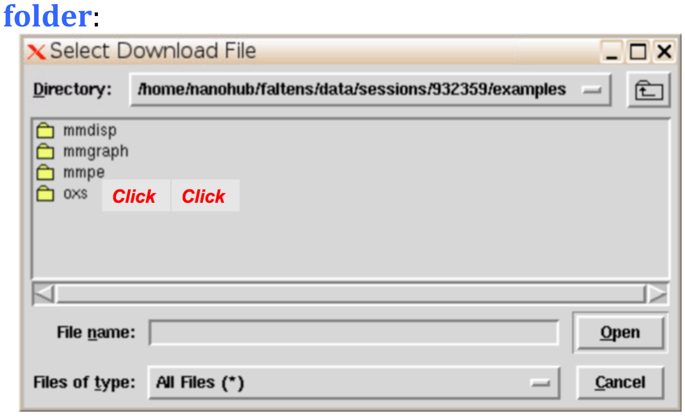
1) If you already have a file to run, **click the "Upload" button** in the *Import/Export* window to transfer the file to your account on the nanoHUB server. If you have many files to upload and download, you can use SFTP. See https://nanohub.org/kb/tips/managefiles.

2) You can alternatively use one of the many pre-loaded example problem files. In order to see what these files contain, open the file using the geany editor, or download a copy to your local machine. You can open and read these files using a text editor or word processing application. To download a file, first **click the *Download* button** in the *Import/Export* window:



A file navigation window will appear. To get to the example file we want, **double-click on the *examples* folder**, then **double-click on the *osx* folder**:

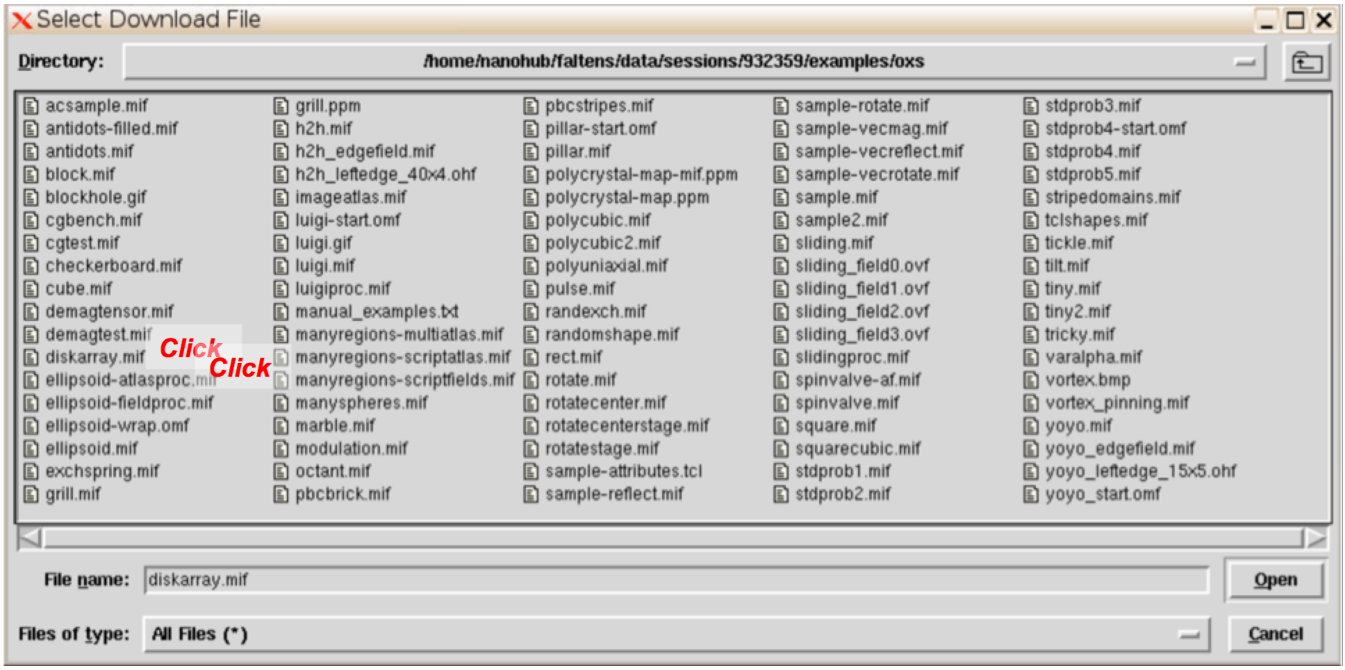




The *oxs* folder contains many *problem files* in the MIF file format. These contain information about the sample geometry, composition, and fields that specify the experiment to be run in OOMMF.

Resize this window so that you can see all the files.

Double-click on *diskarray.mif*, which is the example problem file to be used in this guide:



A pop-up window will prompt you for a location on your local machine to save the example problem file.

You can read *diskarray.mif* with a text editor or word processing document. The file starts,

```
# MIF 2.1
# MIF Example File: diskarray.mif
# Description: Example file using an Oxs_ScriptAtlas to define an array
#  of disks.
#
set pi [expr {4*atan(1.0)}]
set mu0 [expr {4*$pi*1e-7}]

RandomSeed 1

Parameter cellsize        5    ;# Discretization cell size, in nm
Parameter thickness      20    ;# Film thickness, in nm

Parameter disk_diameter  50    ;# Dimension of disks, in nm
Parameter disk_spacing   75    ;# Spacing between disk centers
Parameter disk_xcount     5    ;# Number of disks in x-direction
Parameter disk_ycount     3    ;# Number of disks in y-direction
```

Farther down the page:

```
# Proc that assigns raw point coordinates to regions.  There
# are 3 regions.  Region 0 is the encompassing matrix/universe.
# Regions 1 and 2 form a checkerboard pattern on the array of
# disks, with the disk in the lower lefthand corner being in
# region 1.
```

In this example, there are 15 disks arranged on a 3 x 5 grid in a checkerboard pattern of A disks and B disks that have different properties.

In a nutshell, this MIF problem file sets variables, defines parameters, and contains computational procedures that set up the **structure to be modeled** and the **external magnetic field to be applied over time**.

There is a block of code that specifies the *atlas*, which defines the *regions* over which the simulation will run. There is a block that defines how the simulation region is discretized into a *rectangular mesh*. A block defines the *uniaxial anisotropy*, and the easy magnetization axes for the A disks (x-axis) and the B disks (y-axis). The block that specifies the *Zeeman energy* shows how the applied magnetic field, H, will change over time. There are blocks to specify the *demagnetization energy*, the time *evolver*, and the *driver*. The simulation *stopping condition* and the *initial magnetization* are also specified.

The following section of the problem file specifies the uniform magnetic field applied through the run:

```
Specify Oxs_UZeeman [subst {
  multiplier [expr {0.001/$mu0}]
  Hrange {
     {    0     0 0     1000  100 0    20 }
     { 1000   100 0    -1000 -100 0    40 }
  }
}]
```

Hrange lists the initial and final values of the applied magnetic field along with the number of evenly distributed stages in the range. The *multiplier* is used to effectively change the units. In this example, $\frac{1\times10^{-3}}{\mu_0}$ converts the SI units of A/m into mT. If the components of the magnetic field are given as H = (H_x, H_y, H_z), then this block specifies that the magnetic field will start at an initial strength of H = (0,0,0) mT and evenly increase to H = (1000,100, 0) over 20 stages. Then the field will decrease to H= (-1000, -100, 0) over 40 stages. There will be varying numbers of simulation steps within each stage, which evolves until the sample reaches the *stopping condition*, which is often equilibrium or steady-state.

To learn more about the components of a problem file, refer to the **OOMMF user guide**: http://math.nist.gov/oommf/doc/userguide12a6/userguide/.

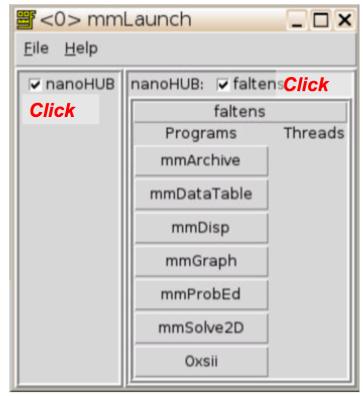
Loading a Problem File and Running an OOMMF Simulation

All of the example problems in the *oxs* directory are already in nanoHUB, but not yet loaded into the OOMMF *oxsii 3D solver* on nanoHUB to be run.

To load the *diskarray.mif* problem file:

3) **Click the nanoHUB checkbox** in the *mmLaunch* window. This expands the window to show your nanoHUB user account.

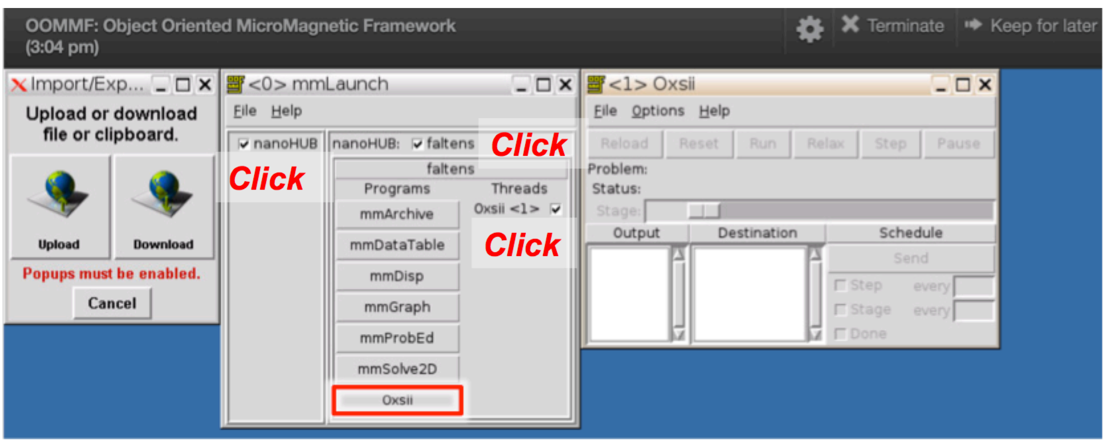
4) **Click the checkbox by your nanoHUB user account**. This will expand the window again, and you will be able to see the 7 Program buttons: *mmArchive, mmDataTable, mmDisp, mmGraph, mmProbEd, mmSolve2D,* and *Oxsii.*



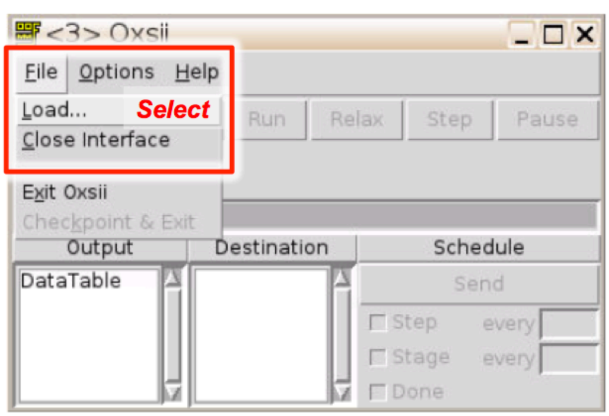
In this guide, we will use *mmDisp*, *mmGraph*, and *Oxsii*. Once you see how these components interact, you can click the *mmDisp* and *mmGraph* buttons first to simplify the overall workflow. This guide will take you step-by-step through a sequence, starting with *Oxsii*, so that you will see the effect of clicking each button.

5) **Click the *Oxsii* button** in the *Programs* column. An instance of *Oxsii* will be launched, and *Oxsii<1>* will be added to the list of threads. *Oxsii* is the OOMMF eXtensible Solver Interactive Interface.

6) **Click the checkbox by *Oxsii <1>*** in the *Threads* column to open a window containing the *Oxsii <1>* interface window:



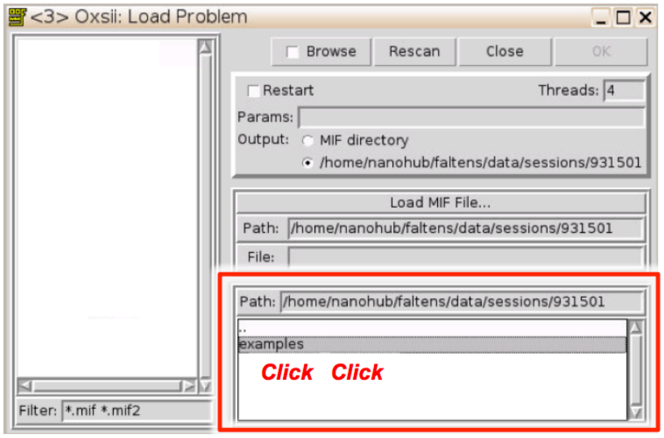
1) From the *File* drop-down menu in the *Oxsii* window, select **Load...**

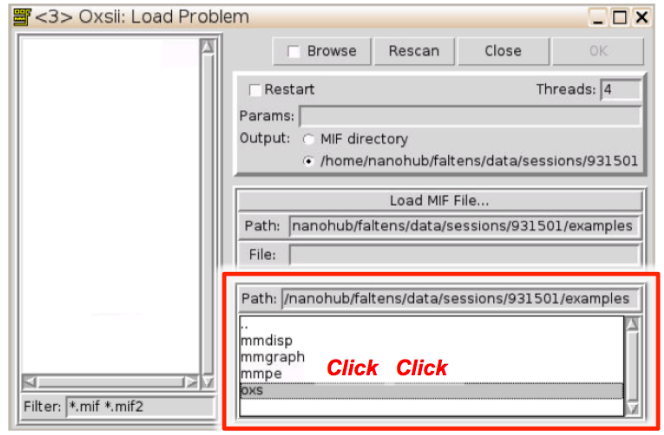


A new window will appear, *Oxsii: Load Problem*.

2) In the lower right corner of the *Load Program* window, **double-click on "*examples*"** to open the examples folder.

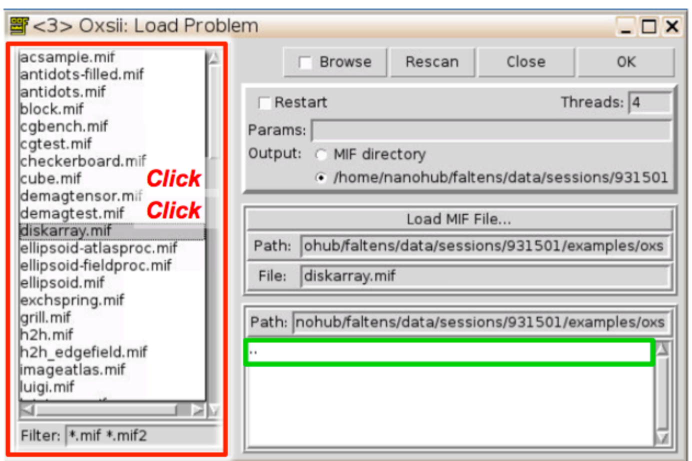
3) There are 4 folders in the examples folder. **Double-click on "*oxs*"** to open the *oxs* folder.





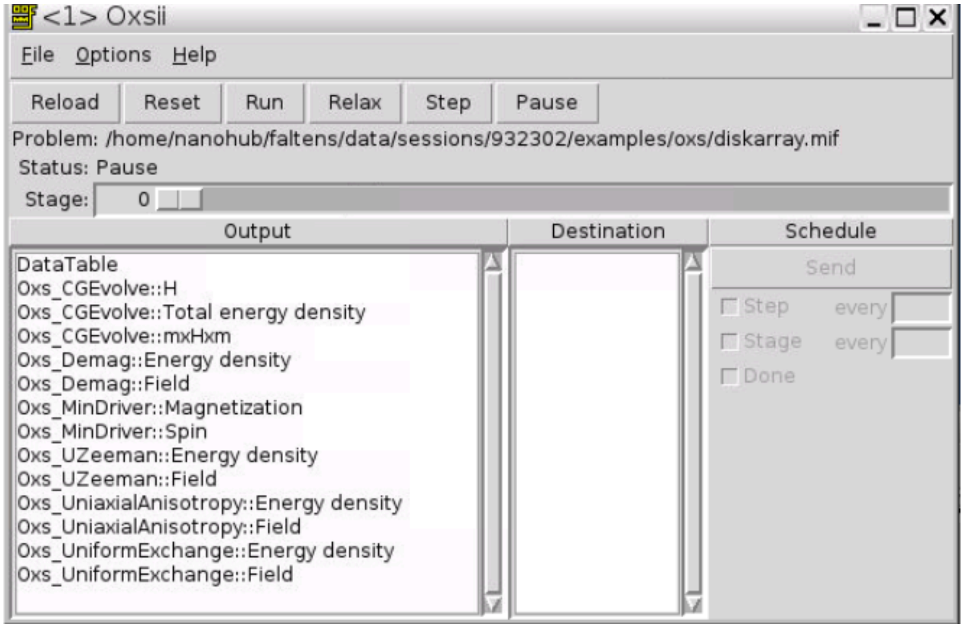
This will display the example files in the left-hand window. If you want to navigate back up a level, click on ".." (outlined in green) in the *Path* frame.

4) **Double-click on the file** you would like to load. This guide uses the file, ***diskarray.mif***:



The *Load Problem* window will disappear, and the *Oxsii* window will now show new information.

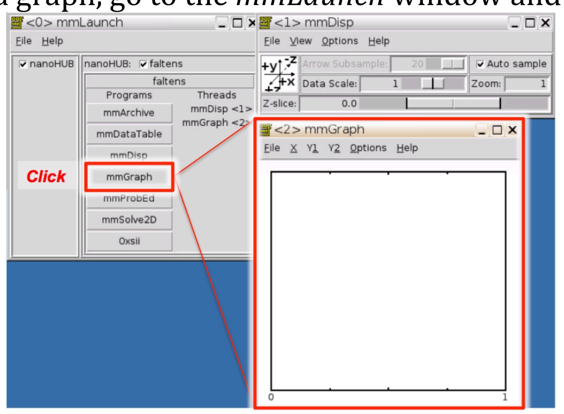
Move and resize the *Oxsii* window so that you can see all of the *Output* available for this particular example. The types of output that are available depends on what is in the problem file. The *diskarray.mif* problem file has 13 types of output. This guide will use two of these, **DataTable** and **Magnetization**.



<u>Viewing scalar data from ***DataTable*** in an *mmGraph* window</u>

In the *Oxsii* window's *Output* frame, **click on *DataTable*.**

Notice that there are not yet any Destinations listed. In order to send **scalar data** from DataTable to a graph, go to the *mmLaunch* window and **click once on the *mmGraph* button.**



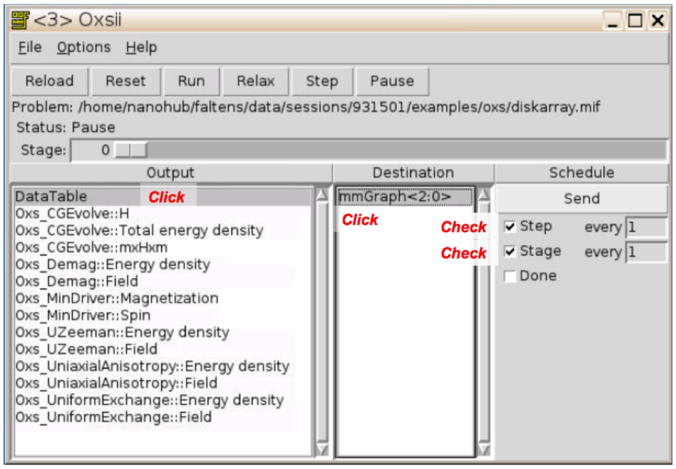
(imagine image does not have mmDisp there already)

An *mmGraph* window will open, and *mmGraph<2>* will be added to the list of *Destinations* in the *Oxsii* window as well as and the list of *Threads* in the *mmLaunch* window.

5) In the *Oxsii* window's *Destination* frame, **Click on *mmGraph<2:0>*.**

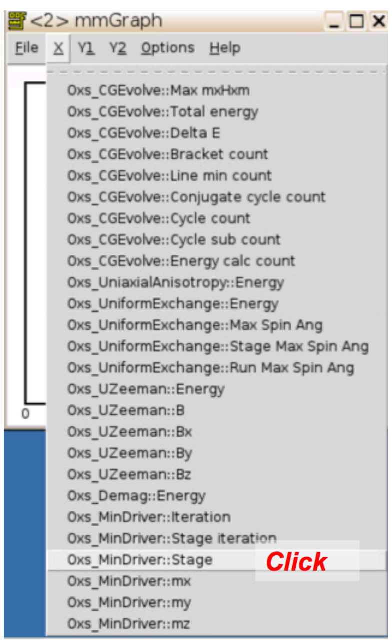
6) **Check the *Step* and *Stage* boxes** that now appear in the *Schedule* frame

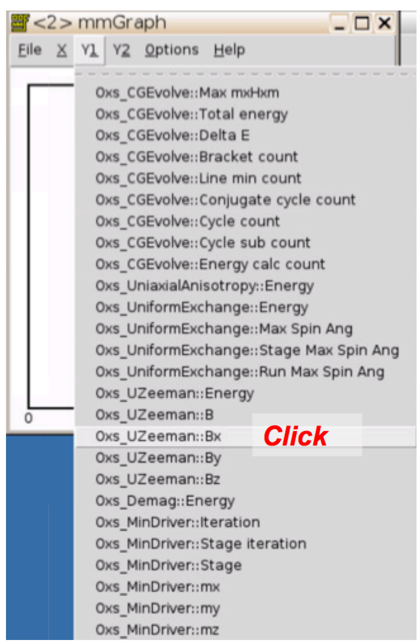
Your Oxsii window should now look like this:

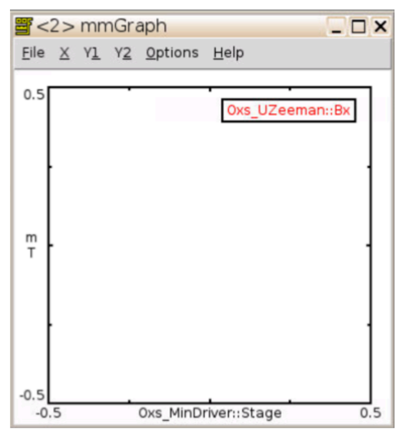


7) **Click on the Send button** to make this information available in the *mmGraph* window.

8) In the *mmGraph* window, select the values to be plotted on the x- and y-axes. For our example: In the X drop-down menu, **click on *stage***, and in the Y1 drop-down menu, **click on *Bx***. You will see Bx (in red) added to the legend in the *mmGraph* window.

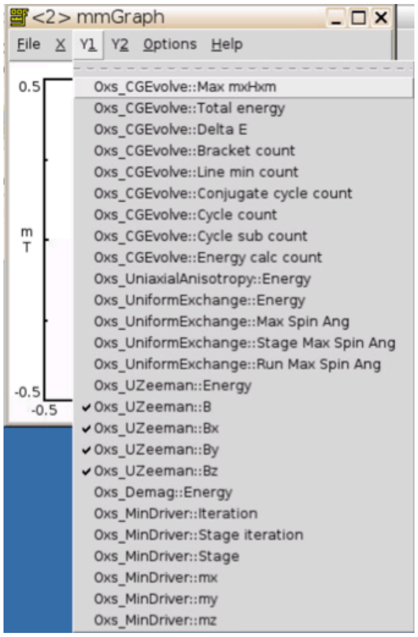


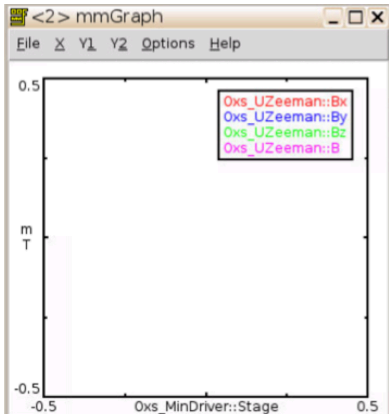




Multiple values can be plotted on one graph. To add By, Bz and total magnitude, B to the graph:

From the Y1 drop-down menu, **click on *By***, then **click on *Bz***, and finally **click on *B***. These values are sequentially added to the *mmGraph* legend, and appear in blue, green, and pink.





The *mmGraph* window is now set up to dynamically display the results of the simulation as it proceeds.

<u>Viewing the vector field ***Magnetization*** data in an *mmDisplay* window</u>

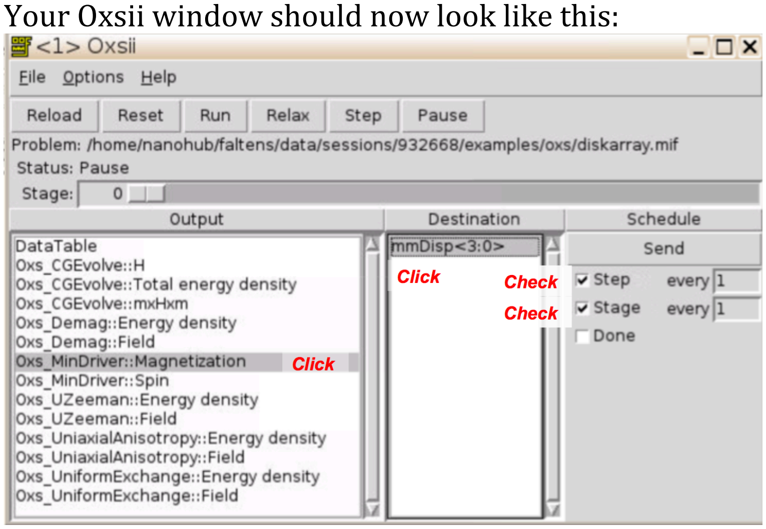
In the *Oxsii* window's *Output* frame, **click on *Magnetization*.** Notice that there are not yet any Destinations listed. In order to send **vector data** from *Magnetization* to a display window, go to the *mmLaunch* window and **click once on the *mmDisp* button.**

An *mmDisp* window will open, and *mmDisp<3:0>* will be added to the list of *Destinations* in the *Oxsii* window as well as and the list of *Threads* in the *mmLaunch* window.

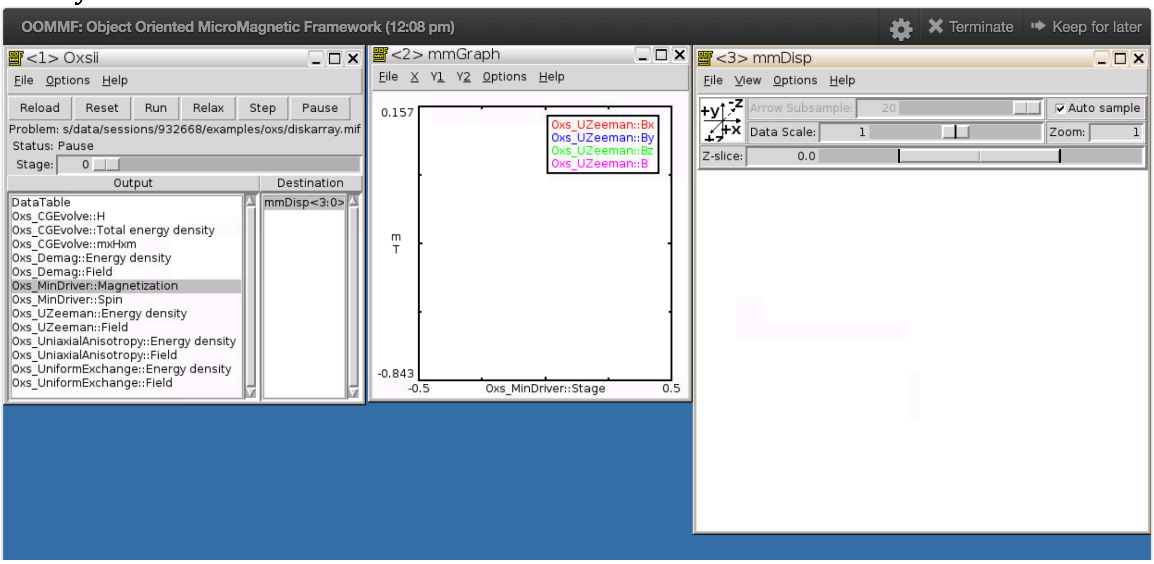
9) In the *Oxsii* window's *Destination* frame, **click on *mmDisp<3:0>*.**

10) **Check the *Step* and *Stage* boxes** that now appear in the *Schedule* frame

Your Oxsii window should now look like this:

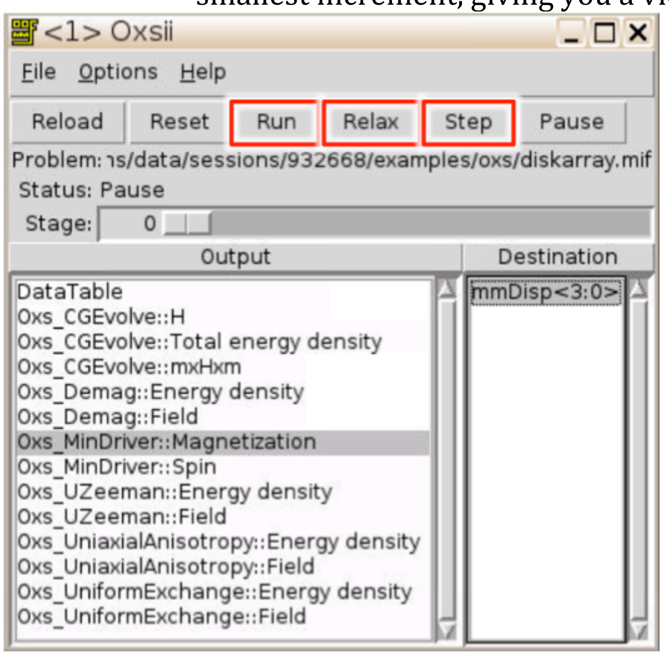


Increase the size of the *mmDisp* window to include an area for the visualization, and position both the *mmGraph* and *mmDisp* windows so they can be easily viewed during the simulation run.
If you have limited screen space, you can minimize windows that are not needed now, such as the *import/export* and *mmLaunch* windows. If you have room on your monitor, you can **resize** the entire OOMMF window by dragging out the bottom left corner of the window. The windows automatically tile as the main window resizes.

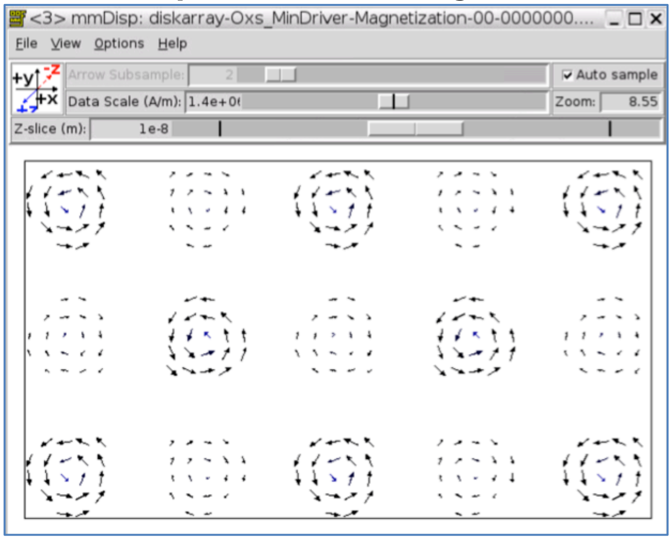


Running the Simulation

1) You have a few choices for running the simulation. In the *Oxsii* window:
    a. **Click the *Run* button:** The program will progress through all of the *stages* of the simulation until the *run* is complete. The current *Stage* is shown in a progress bar.
    b. **Click the *Relax* button:** The program will progress through many *steps* until the current *stage* is complete, then it will *pause* and wait for you to click another button.
    c. **Click the *Step* button:** The program will progress one *step*, then pause. This is the smallest increment, giving you a view of the finest grain of change.



For this example, **click the *Step* button**. The initial magnetization state of the sample will be shown in the *mmDisp* window. This is a good time to resize and move this window if needed.



Click the *Relax* button to let the simulation run to the end of this first stage. While the simulation is running, the Status will be *Relax*. At the end of the stage, the Status changes to *Pause*. You may also see the magnetization vectors moving.

Be sure to watch the dynamically changing *mmDisp* and *mmGraph* windows during the run. As you move from stage to stage through the run, you will be able to see where the sample magnetization saturates, as well the remanent magnetization.

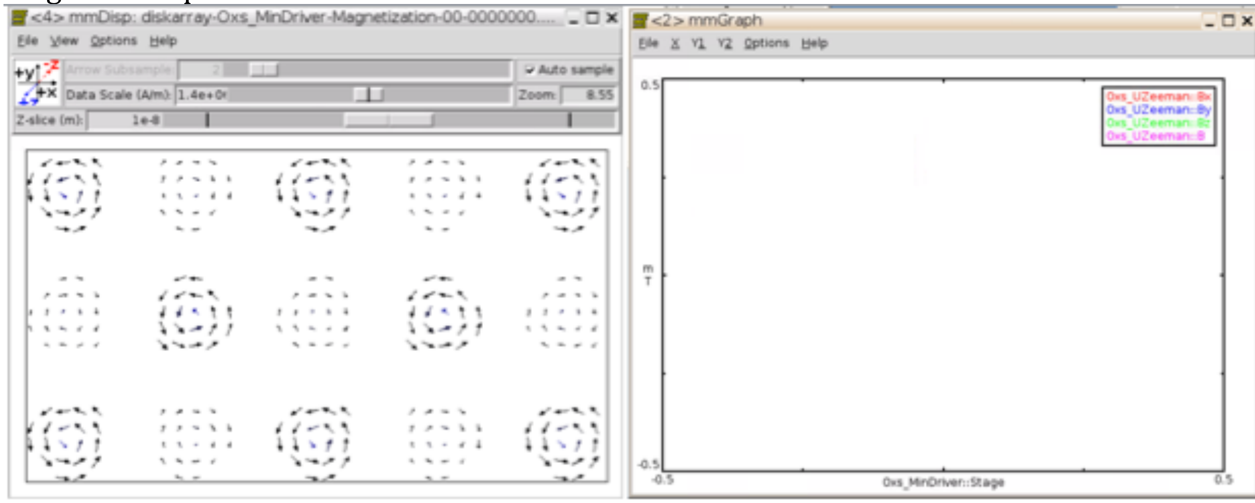
There are additional controls to explore beyond what is explained in this guide. In the *mmDisp* window, the *Z-slice* slider shows cross-sectional views of the sample at various positions along its third dimension. The *Data Scale* can be changed, and the vector magnitude represented by length or color. Clicking different areas in the tricolor X,Y,Z axes button changes the perspective of the display. See the **OOMMF user manual** for details.

To rerun this simulation, in the *mmGraph* window click **Options: Clear Data**. In the *Oxsii* window, **click the *Reset* Button**. You might want to **click the *Run* button** to watch the entire simulation progress without stopping.

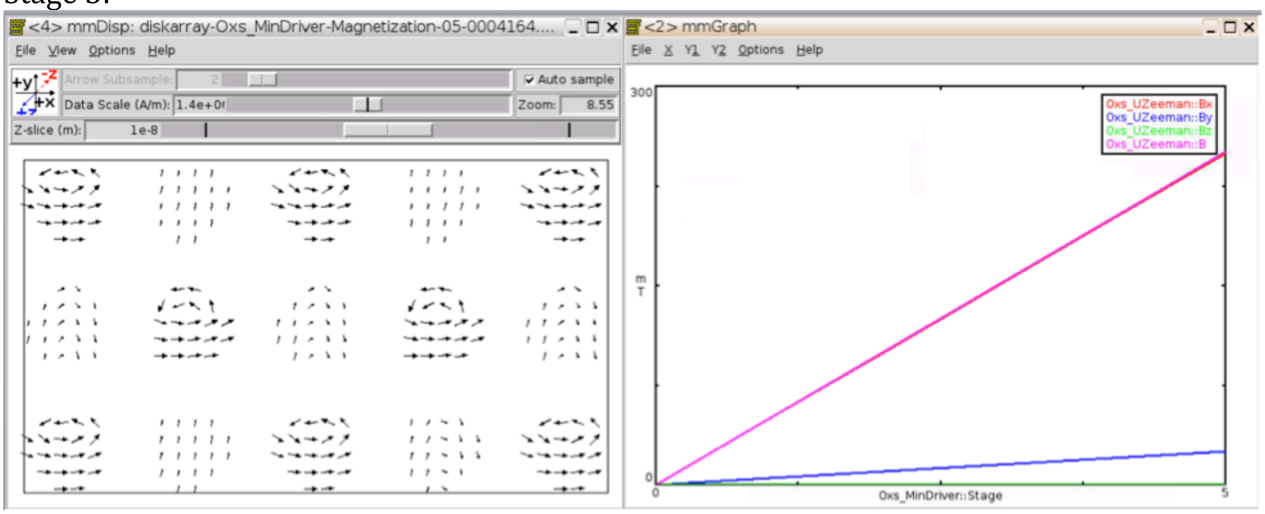
Downloading the data in text format is a two-step process. First save the data to your nanoHUB account, specifying the pathname and filename. Then use the *Import/Export* window to save the data on your local computer.

It may be easiest to capture images by taking screenshots. Following are screenshots taken at the end of selected stages of the simulation run (the *Relax* button was used). The image on the left is the *mmDisp* window, which shows the magnitude and direction of the magnetization vectors in each of the 15 disks. The image on the right is the *mmGraph* window, which shows the components of the applied magnetic field, as well as the total applied magnetic field, as a function of simulation stage. H_x is red, H_y is blue, H_z is green, and the magnitude of the total magnetic field H is pink.

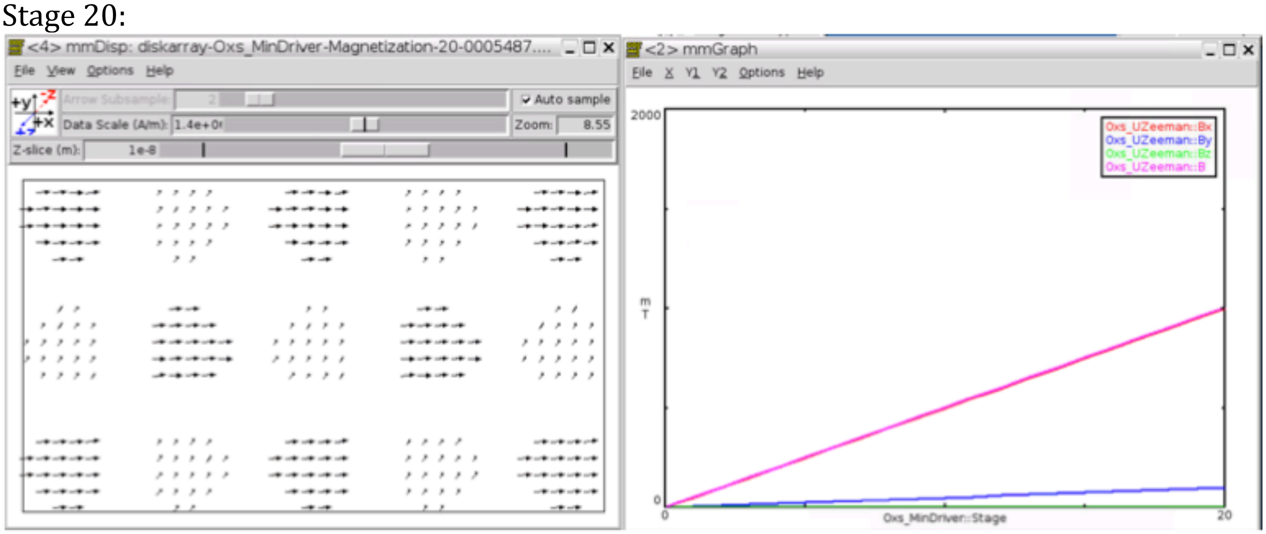
Stage 0: Sample Initial Condition



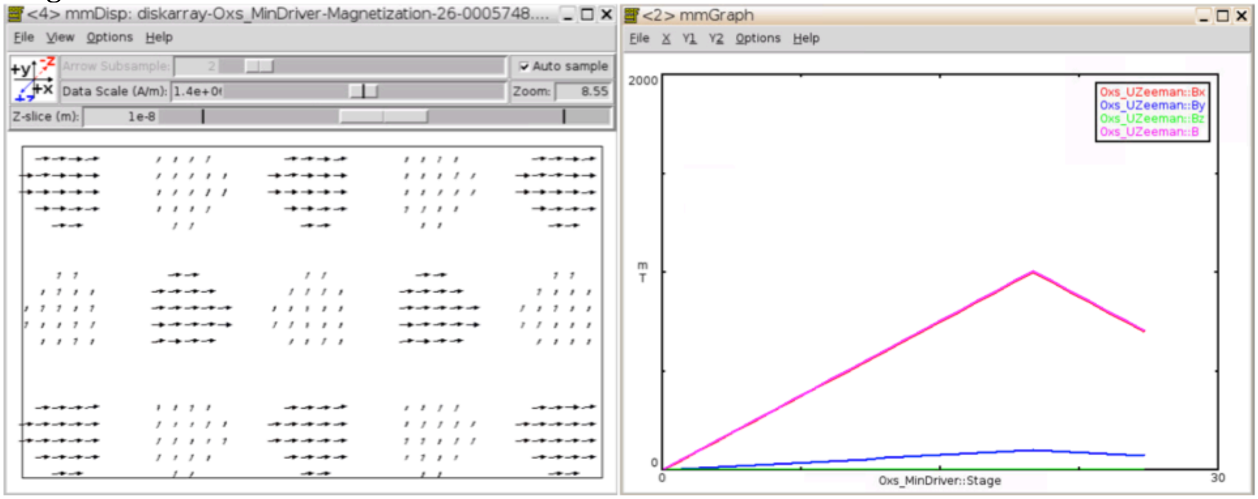
Stage 5:



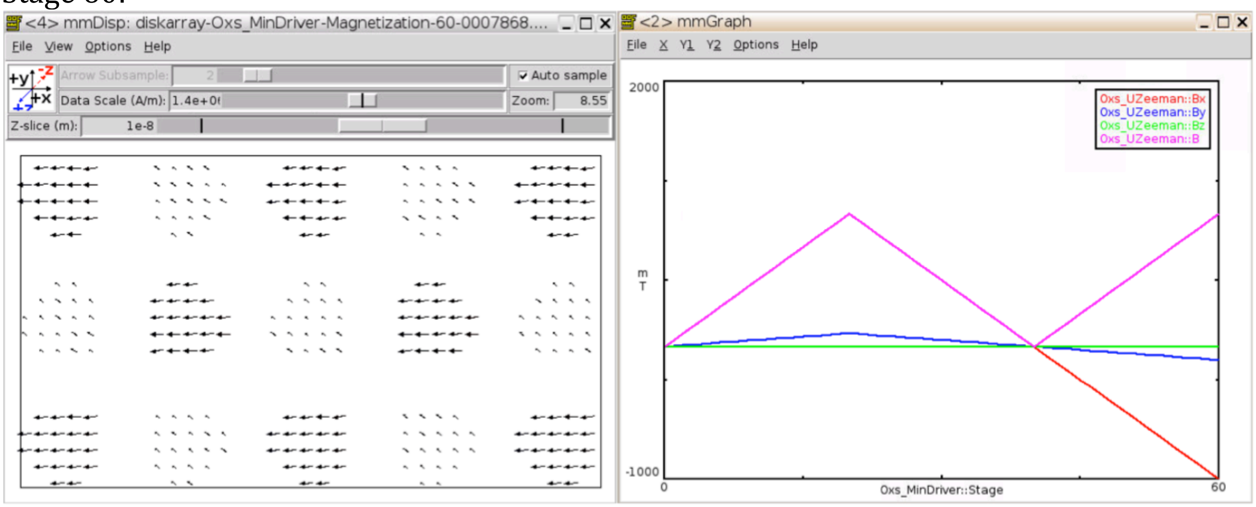
Stage 20:



Stage 26:



Stage 60:



Note: something very cool happens as the sample moves from stage 50-51. Be sure to observe this!

How to get help

From the page where you encountered problems in nanoHUB, click the "Need Help?" link in the upper right hand corner of the window, and include a detailed description of the problem you are encountering. The trouble ticket will be assigned based on the nature of the problem.

References

These materials were instrumental in enabling me to use OOMMF and create this document to share these tips with others.

Many thanks to Dr. J.J. Park at the University of Maryland for walking me through the process of running an OOMMF simulation on the nanoHUB cyberinfrastructure.

OOMMF user guide: http://math.nist.gov/oommf/doc/userguide12a6/userguide/

Online OOMMF tutorials: http://deparkes.co.uk/oommf/oommf-tutorial/

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