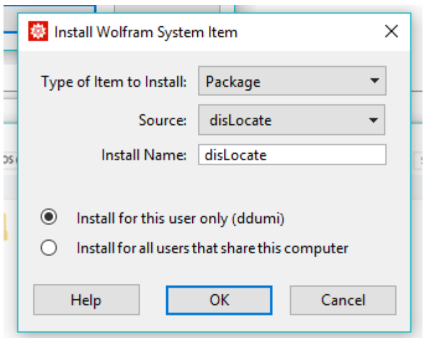
disLocate User Guide

For basic use and understanding

Download *disLocate.m* and *User_Manual_(disLocate).nb*, then open in Wolfram Mathematica. The user manual is a tutorial to introduce you to the different functions available. Follow the instructions to install the package within the notebook.



1. Install the Package:
Menu Bar > File > Install... > Type [Package] Source: [From File...] Name: [disLocate] > [OK]

2. Run all Examples by clicking:
Menu Bar > Evaluation > Evaluate Entire Notebook

Follow step 2 to evaluate all the example cells within the user manual. In Mathematica a cell is a block of input code to be executed.

```
In[3]:= << disLocate`
        disLocateVersion
```

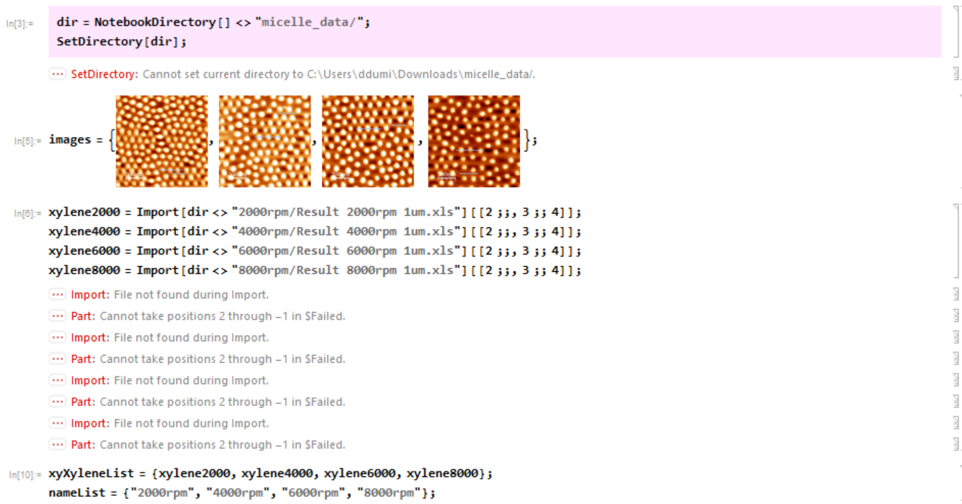
The bracket at the end indicates the size of the code block/cell. To evaluate a single cell press shift + enter.

Troubleshooting Errors:

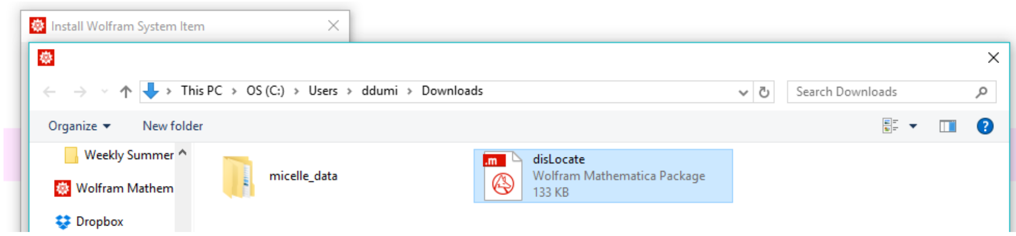
1. C compiler error. If your computer does not have a C compiler this error message will appear. Don't worry, you do not need one to use disLocate. If **disLocateVersion** gives an output, as seen below, then the system is running well.

```
In[3]:= << disLocate`
        disLocateVersion
   x: Symbol x appears in multiple contexts {disLocate`, Global`}; definitions in context disLocate` may shadow or be shadowed by other definitions.
   CCompilerDriver`CreateLibrary: A C compiler cannot be found on your system. Please consult the documentation to learn how to set up suitable compilers.
   Compile: A library could not be generated from the compiled function.
   CCompilerDriver`CreateLibrary: A C compiler cannot be found on your system. Please consult the documentation to learn how to set up suitable compilers.
   Compile: A library could not be generated from the compiled function.
   DiffractionPatternFromPosition: Symbol DiffractionPatternFromPosition appears in multiple contexts {disLocate`, Global`}; definitions in context disLocate` may shadow or be shadowed by other definitions.
   CCompilerDriver`CreateLibrary: A C compiler cannot be found on your system. Please consult the documentation to learn how to set up suitable compilers.
   General: Further output of CCompilerDriver`CreateLibrary::nocomp will be suppressed during this calculation.
   Compile: A library could not be generated from the compiled function.
   General: Further output of Compile::nogen will be suppressed during this calculation.
Out[4]= 1.2017-02-23.nmeth
```

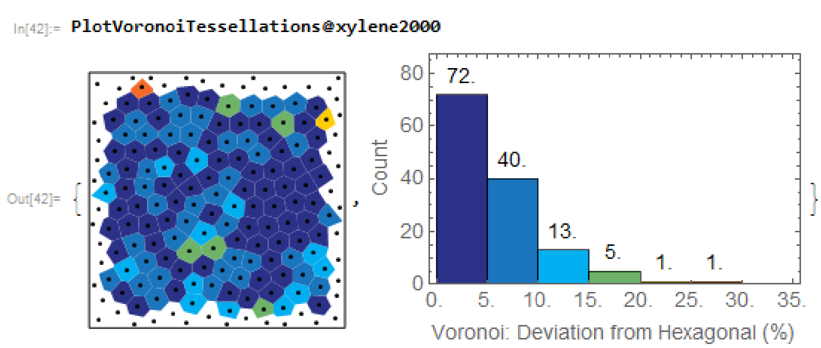
2. After evaluating the entire notebook, all of the functions fail and show error messages. This is likely because the example micelle data file is not located near the disLocate package.



Download *micelle_data* from dropbox and save it in the same folder as *disLocate.m*. Make sure *micelle_data* is unzipped.

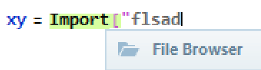


Once evaluated you should get the proper images and graphs. Click on the image and drag the corner to make it larger.



The following addresses what you may encounter once you graduate to using the package with your own data.

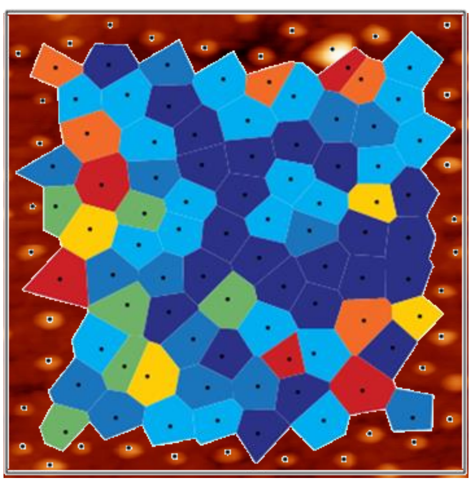
3. Loading files into Mathematica. In newer versions, it may be easier to forget about setting a directory. You can type in **Import ["file path.filetype"]**. Using the file browser that appears once you type into the square brackets, you can search for your file and select it. However this does not work in earlier versions (anything before version 10).



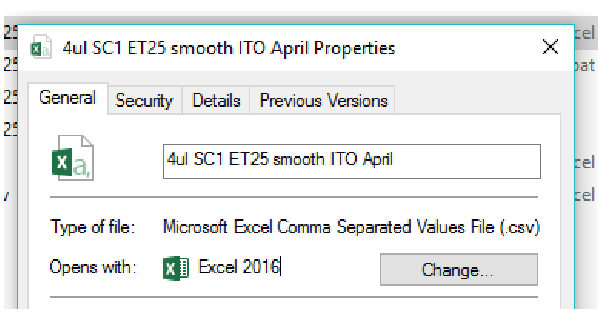

```
xy =
  Import[
   "C:\\Users\\ddumi\\Documents\\Summer 2017\\Research\\Mathematica\\practice data\\4ul SC1 ET25 smooth ITO April.csv"];
```

Don't be afraid to check Mathematica>Help>Wolfram Documentation for assistance.

4. You can overlay the voroni tessellations overtop of the nanoparticle image in Word. Select the tessellation image and create transparent areas, Picture Tools > Recolor> Set Transparent Color. Click the area on the image you want to make transparent. Next you need to invert the tessellation image such that it is upside down and place it over top of the nanoparticle image. It should look like this:

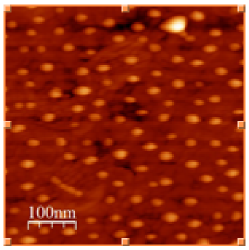


5. This package may not work with .xls files. When saving spreadsheets, save them as .csv. You can check the file type by right clicking on your file and selecting properties.



6. Importing images is the same as importing a file. Create a variable for your image and use the file browser to search for your image.

```
img =
 Import[
  "C:\\Users\\ddumi\\Documents\\Summer 2017\\Research\\Mathematica\\practice data\\4ul SC1
    ET25 smooth ITO April Image 1.jpg"]
```



Data Analysis:

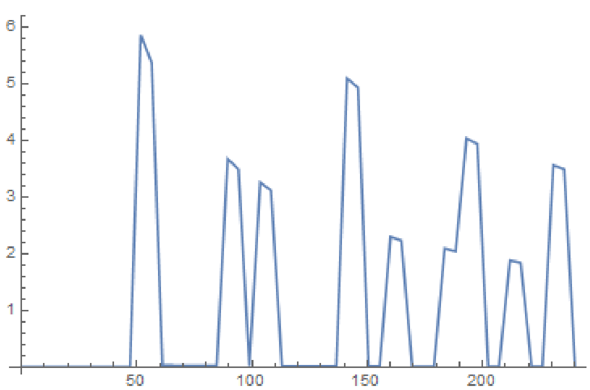
The Pair Correlation Function shows us the probability of finding particles at a radius from a central particle. In the tutorial, xy-coordinate data (of a micelle distribution) is compared to a hexagonal packing order.

To compare your data to the hexagonal order, you can use the function HexagonalLattice[ ] (*since this is a function you must always remember to include the square brackets*).

Here we have the plot of our pair correlation function for the hexagonal lattice.

```
In[27]:= ListLinePlot[PairCorrelationFunction[
           HexagonalLattice[box → rectangleBindingBox[1000, 1000]]], PlotRange → All]
```

Out[27]=



This graph appears automatically as the green dotted line for comparison.