

## Basic Installation

Download from <https://www.enthought.com/products/canopy> either the free or academic version of Enthought Canopy. Your Python version must be 2.7 or newer.

Method 1:

- Install by running `git clone https://github.com/samedling/MCSAS.git` to download the entire repository.
- For future updates, run `git pull origin master` from the MCSAS folder. You may also need to manually remove your old `fastmath.so` file.

Method 2:

- Go to <https://github.com/samedling/MCSAS> and click Download ZIP in the lower right to install. Update the same way.

There are two optional but recommended ways of speeding up the code:

1. (Strongly recommended:) Install PyOpenCL following the directions at <http://wiki.tiker.net/PyOpenCL/Installation> and then the first time you run it, it will ask you which platform and device you want to use. Try the GPU first; if it doesn't work, use the CPU. On my dual core CPU, I obtained a 25x speedup (and during fitting enabled another 5x speedup for a total of ~125x); quad core CPUs should be nearly twice as fast and GPUs should be even faster!
2. F2Py acceleration should work automatically on OS X or Linux. If not, or if you want to make sure you get every bit of performance you can and you have gfortran installed, run `make` to compile the Fortran code (or if you have ifort installed, edit the makefile before running `make`). I've found this useful even if you are running OpenCL on the CPU (it might be unnecessary if running OpenCL on the GPU). On my dual core CPU, I obtained an 8x speedup (and during fitting another 10x speedup for ~80x); quad core CPUs likely not much faster. There is a small benefit to having this in addition to OpenCL.

Run `python newgui.py` on the command line or open it in Canopy and click run. (Note: you may discover running `nice python newgui.py` results in your system being a lot more responsive.)

If you want to try out the latest features, you can try the develop branch (by either running `git pull origin develop` or via the web GUI clicking on 'master', selecting 'develop', and then downloading the zip) but consider editing `global_vars.py` so `debug = False`.

## OS X Fortran Installation

Apple doesn't provide a recent version of gfortran, but you can download one from <http://hpc.sourceforge.net>

If you also don't have Xcode Tools, follow the directions at <https://wiki.helsinki.fi/display/HUGG/Installing+the+GNU+compilers+on+Mac+OS+X>

1. Install XCode Tools from the App Store.
2. Install the Command Line Tools by running `xcode-select --install`
3. Download the latest stable gfortran version from <http://hpc.sourceforge.net>

Tested on OS X 10.10 "Yosemite".

## Some Troubleshooting

If things ran fine before, but after updating returns `KeyError`, remove the file called

default.txt.

OS X and Windows: You need to close all the old plots before you can run things again. Otherwise, it's otherwise unresponsive for some reason.

OS X/EPD/Tkinter: Make sure you have Canopy. EPD might tell you it's updated everything, but it's still not the same as Canopy.

If you receive compiler OpenCL compiler warnings when starting the program it's probably due to your OpenCL device not supporting 64-bit floating point numbers; it should be fine, but if you get errors later, try using a different OpenCL device.

Linux/OpenCL: apt-get on Ubuntu wasn't helpful to me; follow the directions linked above for more success.

PIL: On older systems you may need to manually remove PIL and install Pillow (sudo pip uninstall PIL and sudo pip install Pillow); newer systems should simply come with Pillow. Otherwise Image won't be able to read the funny SAXS TIF files.

Scientific Linux/F2PY: Make sure you are using the version of F2PY which matches your version of Python (2.7+), otherwise just loading the Fortran module causes a Segmentation Fault.

Fortran/Hyperthreading: If you have a Core i7 processor, (or other CPU with hyperthreading) performance may be slightly improved by adding `export OMP_NUM_THREADS=<n>` to your `.bash_profile` (where `n` = the number of physical cores).

Due to the large number of shapes, it's possible some of the sped-up versions of these have bugs. If you find that the shapes don't look right, edit the `global_vars.py` file so `accelerate_points = False` to disable the erroneous speedup.

## Running the Program

### Individual Monte Carlo Calculations

After selecting the Monte Carlo model, pressing the Parameter Help button will rename individual model parameters to be more descriptive and grey out unused parameters.

'Real Space' will show you the points.

'Calculate Intensity' will show you the detector image.

To activate the advanced options, click on the Pop-Up Window buttons at the right.

If the Save Images box is checked it automatically overwrites anything with the same filename.

- The Radial Symmetry checkbox speeds the program, so check if appropriate.
- Neighboring point distance and z-direction scaling can provide speedups at the expense of decreased background contrast; doubling the neighboring point distance decreases the number of points by a factor of 8, while doubling z-direction scaling decreases it by a factor of 2.
- Opening multiple copies of the same window is not recommended. If you do, it will use the values in the one you opened most recently but it will constantly reopen uneditable old ones. Or sometimes it will produce an error until you close them and reopen one. Either way you'll get confused, so avoid opening more than one of each window.
- Taking into account a non-infinite coherence length really complicates things. By default, the code uses a rough approximation where the object is broken into chunks. This should work reasonably well, but if you want to really calculate it the long way, there's a button

for that in Detector Options and I recommend no more than 2500 (50x50) pixels and 5000 points if you want it to take less than an hour.

## Performing Fits

1. Input the name of the experimental data file to fit and click "Plot Exp Data". If "Center of Beamstop" is left blank ("0 0") then it will plot the original experimental data (which takes a minute). The lower bounds option in the center column is quite useful here. Try a value in the range  $1e-8$  to  $1e-6$ . Then, move the mouse over the center of the beamstop and read the x,y-coordinates from the plot screen. Use these values and replot the experimental data. It will crop a square around the center and downsample it so the side length is equal to the Pixels parameter.
2. Input known values, uncheck relevant parameter boxes, make a good guess of unknown parameters. To see how good your guess is, press "Plot Residuals".
3. When you have a satisfactory guess, click "Fit Exp Data". Each iteration, it prints out the time and the sum of the residuals; be aware that it is normal for the sum of the residuals to go several iterations without changing significantly.
4. Read the fit results from the terminal. If you had a grid compression  $>1$  (assuming you're using Fortran acceleration) and now you want more printable results, copy the fit results back into the GUI and Plot Residuals.

Some comments: *Grid compression only works reliably with Fortran; it works with OpenCL if the number of points/pixels does not exceed OpenCL's capabilities.* If the fit steps are each taking less than 10 seconds, there would probably be very little additional time taken by increasing pixels by 40% or halving the grid compression or  $z\_scaling$ . *Be careful when letting the background vary. If the background gets set too high by the computer, it cannot normalize properly and all bets are off.* Checking the radial symmetry box decreases the time taken by 30-50% (30% for Fortran, 40% for OpenCL, 50% for pure Python).

## Adding Models

First, make sure you have the most recent version.

### To add a Monte Carlo model:

Open `density_formula.py`

1. In `density(coords)`, at the top, created another `elif` line at the bottom like all the others.
2. Add an element to the end of `g.model_parameters`. Note, you'll need to put a comma at the end of the previous last line and then put in useful descriptors for each of the parameters you are using (to show the user when they click the help button). (Do not add to the middle of the list as this will cause errors when Fortran or OpenCL are enabled.)
3. Create a new density function `d###name` near the bottom using one of the two templates at the very bottom.

Save and close the file.

Optionally: If you want to speed up the calculation using Fortran, edit `fastmath.f90` with a Fortran version of your new density and edit the `elif` blocks in `Points_For_Calculations()` in `Monte_Carlo_Functions.py`. If you want to speed up the calculation using OpenCL, edit `density.cl` with an OpenCL version of your new density and edit the `elif` blocks in `opencl.py`, `class OpenCL`, `def density()`.

### To add an analytic model:

1. Open `analytic_formula.py`. Near the bottom of the file but above where `theory_csv` is defined, create another `"elif:"` block like the ones above it. Remember the number you

- assigned. Save and close the file.
2. Open newgui.py and go to the line defining Analytic\_options. After the last number (currently around line 90), add a line like the ones above it using the number from step 1. Save and close the file.

Finally (after some testing), use git to add/commit/push (see below for details) or e-mail a collaborator to do it for you.

## Uploading Changes with Git

### Git Setup

Make sure you have git and a github account.

E-mail [scott.medling@anu.edu.au](mailto:scott.medling@anu.edu.au) with your username so I can add you as a collaborator.

Optionally, to configure your local git, run

```
git config --global user.name "<Name>"
git config --global user.email "<E-mail Address>"
git config --global color.ui auto          #Improves readability.
git config --global core.editor vim        #If you like vim.
```

To download the respository, run

```
git clone https://github.com/samedling/MCSAS.git
```

### Basic Git Use

Every time you edit

```
git pull origin master    #Download latest changes.  Run every time you start.
```

After editing a file, or number of files

```
git add <filename>        #Adds a filename
git add <filename2>       #Adds another filename, etc.
```

```
git status                #Tells you which files have been changed/added.
```

```
git commit -m "<Insert short message here.>" #Saves added changes locally.
git push -u origin master #Uploads committed changes to respository.
```

### Other Useful Git Commands

```
git log --oneline         #Displays summary of each commit.
git log -<n>              #Displays last n commit details.
git log --after="<yyyy-mm-dd>"
```

### Advanced Git Use

If there's a collision/conflict/whatever (usually at the push stage) because you and someone both editing the same part of the same file, you'll need to manually fix it, which sometimes sucks. You may need to separately run

```
git fetch origin master
git merge
```

If you want to go back just to look, make sure you've committed any changes and then run

```
git checkout <hex_number>
```

To create a new branch so you can make commits based on an older version (again, make sure you've committed any changes), run

```
git checkout -b <branch_name> <hex_number>
```

For potentially unstable changes, use the develop branch:

```
git checkout -b <branch_name>    #Creates branch from current commit.
git checkout develop              #Switch branches.
```

Make your changes, commits, etc. Then merge:

```
git checkout master              #Switch back to master.
git merge develop --no-ff        #Merge while preserving commit history.
git push
```

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