Manual for ModelScanning3DXRD.py v. 1.0

-a casual guide for a general use case

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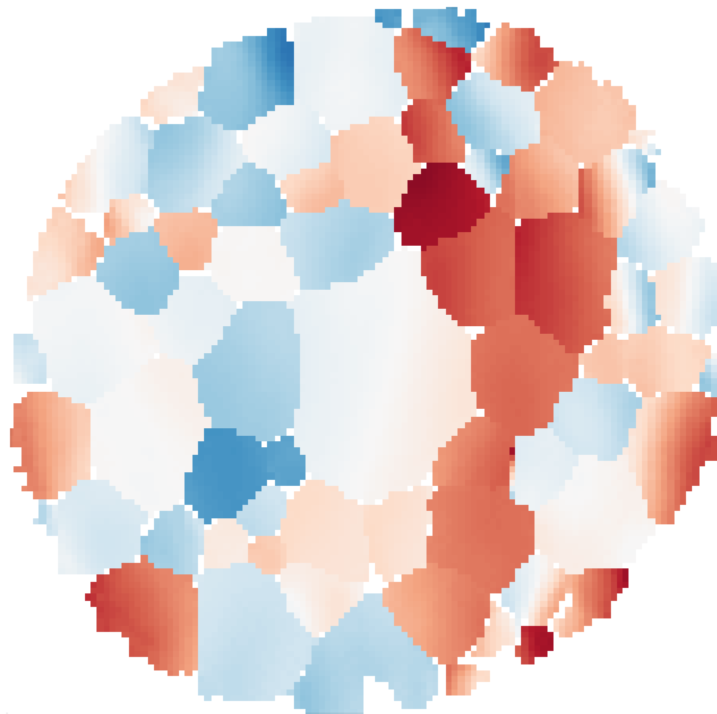

This is a casual manual to use and understand the code for ModelScanning3DXRD.py.

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Background

The central ideas of Scanning-3DXRD is described in Hayashi et al. (2015) and Hayashi et al. (2017). The goal of the here provided algorithm is to forward model a diffraction pattern based on a per-voxel definition of the sample. This means that the sample is built up from a number of cubic voxels with side equal to the beam size. Each voxel can carry position, orientation and strain. Currently, the main use case for the forward model is to evaluate the accuracy of various reconstruction techniques.

The model that exists in this repository is called ModelScanning3DXRD and was derived from PolyXSim which is documented at `sourceforge.net/p/fable/wiki/PolyXSim/`. The documentation for PolyXSim applies in general to ModelScanning3DXRD.

In general, the reader will have to know her or his way with python, Linux, the general theory of 3DXRD and file formats used for 3DXRD at the ESRF. The code is, and was, developed for scientific use and is not the most user friendly so to speak. This means that apart from reading this handy dandy manual, you will most likely end up doing some trial and error runs.

ModelScanning3DXRD has been used , by the author, with success as described in Henningsson (2018). In the thesis the reader may find more details regarding the background and use case. The thesis can be found at git-hub (`https://github.com/FABLE-3DXRD/S3DXRD`) at the same location where this document can be found. If not, it is intended to be included in the repository as soon as possible.

Getting Started

To forward model a diffraction pattern the user must supply an input file to ModelScanning3DXRD.py. The input file is a text file that defines the sample and experimental setup. The format of the input file is mostly described at (`sourceforge.net/p/fable/wiki/PolyXSim%20-%20input/`). The main differences are that the keyword "voxel" is used instead of "grain" and that the user must supply a map that maps the voxels together and defines the grains. The reader should be aware of that not all (read: quite few) features originally included in PolyXSim has been tested in ModelScanning3DXRD, and thus you are expected to encounter bugs moving away from the standard use cases described in the example below.

In order to run ModelScanning3DXRD the user must set up their environment in the same fashion as is done for ImageD11, PolyXSim, etc. Documentation for this can be found at the git-hub page. After this is done the user must also install xfab, ImageD11 and FitAllB. Potentially only xfab is needed but you might as well get all the goodness while your at it.

Assuming that you have a conda version of python installed (`https://conda.io/docs/user-guide/install/linux.html`) the following series of commands will hopefully work (tested with a Ubuntu distribution).

```
sudo apt-get install git-core
conda create -n fable python=2.7.15
source activate fable
conda install numpy scipy pillow matplotlib ipython scikit-image h5py
pip install fabio --no-deps
pip install cython
pip install pmw
pip install pyopengltk
cd ..
mkdir fable
cd fable/
git clone http://github.com/FABLE-3DXRD/xfab
git clone https://github.com/FABLE-3DXRD/FitAllB.git
```

```
git clone http://github.com/FABLE-3DXRD/PolyXSim
git clone http://github.com/FABLE-3DXRD/ImageD11
git clone http://github.com/FABLE-3DXRD/fabian
git clone https://github.com/FABLE-3DXRD/S3DXRD.git
cd xfab
python setup.py build install
cd ../FitAllB/
python setup.py build install
cd ../PolyXSim/
python setup.py build install
cd ../fabian/
python setup.py build install
cd ../ImageD11/
python setup.py build install
cd ../S3DXRD/ModelScanning3DXRD/
python setup.py build install
```

You could try and run the `tests.py` file located in `S3DXRD/ModelScanning3DXRD/test_voxelated/` to see if everything is healthy.

```
python tests.py
```

The test will take approximately 60 seconds to run and should output all OK for three tests at the end.

Example

We will now simulate the diffraction pattern of a single grain located at the origin. The grain is composed of five by five voxels which all have the same orientation. The strain is varied to simulate a gradient across the grain. The input file always defines a slice in the sample, and to simulate a three dimensional structure several input files have to be produced and simulations run for each of them. The first thing to put in the input file is information of how we want to save our data

```
direc 'Tin'
stem 'Sn_diffrac'
make_image 0
output  '.flt' '.gve' '.par' '.ubi'
```

This will save the output in a folder named `'Tin'` with the base file name `'Sn_diffrac'`. Files of the types `'.flt''.gve''.par''.ubi'` will be saved. We may now specify the nature of the studied material via a `.cif` file as

```
structure_phase_0 '<absolutr file path to .cif file>'
```

For more information on crystallographic input files the reader is refereed to google :). Also the reader may find one or two examples of crystallographic input files in the repository for reference. They are basically text files that specify unit cell parameters atomic type etc.

Now it is time to specify the experimental setup. For information on the below keywords go to the PolyXSim documentation at (`https://sourceforge.net/p/fable/wiki/PolyXSim%20-%20input/`)

```
y_size 0.0500
z_size 0.0500
dety_size 2048
detz_size 2048
distance 162.888383321
tilt_x -0.00260053595757
tilt_y -0.00366923010272
tilt_z 0.00463564130438
```

```
o11 1
o12 0
o21 0
o22 -1
noise 0
intensity_const 1
lorentz_apply 1
beampol_apply 1
peakshape 0
wavelength 0.21878
beamflux 1e-12
beampol_factor 1
beampol_direct 0
dety_center 1048.20100238
detz_center 1041.55049636
omega_start 0
omega_end 180
omega_step 1.0
omega_sign 1
wedge -0.0142439915706
gen_size 1 -0.001240713 0.00000100.000000000
sample_xyz 0.006000.006000.003000000
gen_U 0
```

We also specify the width of the beam as

```
beam_width 0.001000000
```

This means that the beam has a square cross section with the side of 0.001 mm.

Now we must define the sample on a per-voxel basis. This is done by specifying each voxel position and state as:

```
pos_voxels_0 -0.00200-0.002000.000000000
U_voxels_0 1.000 0.000 0.000 0.000 1.000 0.000 0.000 0.000 1.000
eps_voxels_0 -0.0200 0.000 0.000 0.000 0.000 0.000
```

After listing all the voxels from zero to the total number of voxels we specify the total number of voxels as

```
no_voxels 25
```

Then we map each voxel to a grain by inputting the dictionary as

```
voxel_grain_map {0:0,1:0,2:0,3:0,4:0,5:0,6:0,7:0,8:0,9:0,10:0,11:0,1
2:0,13:0,14:0,15:0,16:0,17:0,18:0,19:0,20:0,21:0,22:0,23:0,24:0}
```

the format is here:

```
{voxel_number:grain_number, voxel_number:grain_number, voxel_number:grain_number,...}
```

Such that the above example maps all 25 voxels to a single grain labelled with 0.

We may now run the forward model with the input file as

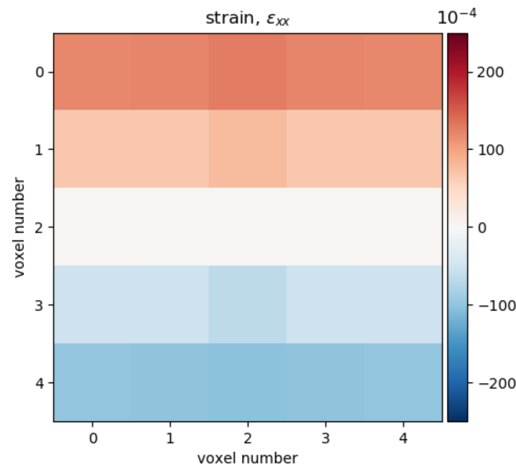
```
python ModelScanning3DXRD.py --input <path to input file>
```

This will run the simulation and printout the progress to the active terminal window. You should see something like

```
Write voxels file
Write res file
Write UBI file
Write detector.par file
Determine reflections positions
no of voxels  25
Done approximately   7 voxel(s) of  25
```

As the simulation finished it will save any output files to the directory specified in the input file. The files are of the same format as those which can be retrived at beamline ID11 at the ESRF.

After deploying some preferred reconstruction algorithms it is possible to receive geometries that reassembles the input sample state. The below reconstruction was retrieved with FBP and a per-voxel local refinement.



Extra Features

For large samples it is recommend to use the "parallel" keyword as an additional input to ModelScanning3DXRD.

```
python ModelScanning3DXRD.py --input <path to input file> --parallel
```

ModelScanning3DXRD will then start several parallel threads for computing the diffraction patterns. In general, for any sample with say 100+ voxels, it is worth while to use the parallel keyword. You will see which voxels are treated by which thread

```
Write voxels file
Write res file
Write UBI file
Write detector.par file
Determine reflections positions
Distributing voxels over cpus
Average number of voxels per cpu:  28.1666666667
Started paralell process for voxel number:  0  to  28
Started paralell process for voxel number:  28  to  56
Started paralell process for voxel number:  56  to  84
Started paralell process for voxel number:  84  to  112
Started paralell process for voxel number:  112  to  140
Started paralell process for voxel number:  140  to  169
no of voxels  169
Done approximately  51 percent
```

ModelScanning3DXRD also has a profiler mode for anyone who wants to try and make the algorithm run faster. You can run in profiler mode as

```
python ModelScanning3DXRD.py --input <path to input file> --profile
```

This will run the algorithm and save a file with statistics. The file will look something like this

```
2030420 function calls in 6.512 seconds

   Ordered by: cumulative time
```

```
 ncalls  tottime  percall  cumtime  percall filename:lineno(function)
      1    1.361    1.361    6.512    6.512 find_refl.py:69(run)
  36450    1.395    0.000    1.917    0.000 find_refl.py:350(find_omega_general)
  82182    0.832    0.000    1.396    0.000 find_refl.py:422(det_coor)
  35800    0.746    0.000    0.970    0.000 find_refl.py:447(calc_int_mod)
 689978    0.806    0.000    0.806    0.000 {numpy.core.multiarray.dot}
 416389    0.597    0.000    0.597    0.000 {numpy.core.multiarray.array}
```

The relevant colon is here the cumtime, which states how much time was spent executing respective function in total.

Pitfalls/Limitations/Bugs

Like mentioned earlier, not all of the extensions used in PolyXSim has been tested with the modified code. The model used at the writing time (November 16, 2018) is fairly simple. Especially the calculation of the intensity is heavily simplified, basically the structure factors and voxel beam overlap is used. Future versions should take more physics into account.

Another simplification is the fact that peaks are assumed to never overlap and that the detector is assumed to have an infinite resolution. This means that the .flt file gets huge since what would normally be a single peak might be many many many delta peaks clustered together. Work is currently put into taking detector pixel size into account and computing peaks as centre of mass of continuous regions of intensity. Hopefully this feature will arrive in a near future. If the .flt files get to big, the reader might want to throw some python code together to parse and split the .flt into several files in order to be a able to read them into matrix format without running out of RAM.

In general more details on the used assumptions and how the algorithm can be used is found in the thesis (Henningsson 2018). The thesis will be made available at the git-hub page as soon as possible. Most likely it will be up before the end of January 2019.

Finally a general disclaimer is announced, as the user may very well find flaws (and hopefully will) and bugs throughout the code. Together we can build something that keeps getting better and better, both from a physics perspective, discussing how these models should be built, as well as from a coding perspective, writing better and more solid code together.

Develop and Adapt

In reality any one who reads this will probably need to modify the code for their specific scientific use. To run the altered code you will need to first run the

```
python setup.py build
```

command, followed by the

```
python setup.py install
```

command. This make sure that the python interpreter is importing the updated modules and not uses the old ones.

Mostly it is the `find_refl.py` script that contains the diffraction model algorithm while the other scripts deal with file handling, parallel runs, input parsing etc. If you would like to improve the model/adapt it this is most likely the place to add some code.

References

Hayashi, Y., Hirose, Y., and Seno, Y. (2015). Polycrystal orientation mapping using scanning three-dimensional X-ray diffraction microscopy. *Journal of Applied Crystallography*, 48(4):1094–1101.

Hayashi, Y., Setoyama, D., and Seno, Y. (2017). Scanning three-dimensional x-ray diffraction microscopy with a high-energy microbeam at spring-8. *Materials Science Forum*, 905:157–164.

Henningsson, N. A. (2018). 3dxrd reconstructions for intragranular resolution - a forward model for scanning-3dxr.