# Dictionary indexing tutorial

This guide will walk you through how to perform a dictionary indexing run using EMsoft and the MATLAB packages in EMsoft-utilities.

It assumes data was acquired by an EDAX system, with orientation data in an .ang file and patterns stored as individual images labeled _00000, _00001, etc. If not, some steps may be different, and EMsoft-utilities is not currently able to handle other data formats. If you would like to use EMsoft-utilities and have data stored in a different format, feel free to contact me and I can try to make code modifications (or feel free to modify the code yourself, it shouldn't be too difficult).

Last revision 3/10/20 (Edward Pang, MIT)

## A. CREATE MASTER PATTERN

**You only need to do Step A once for a given material/voltage/sample tilt angle combination.*

### i. Create an .xtal file to define the crystal structure

**You only need to do this step once for a given material. If you want to simulate a new voltage or sample tilt angle for the same material, skip to step ii.*

1. From any location, run the EMmkxtal program.

```
jonathan@X99:~/epang/EMsoftfiles$ EMmkxtal
```

2. Answer the series of prompts to fill in the unit cell information. The .xtal file will be automatically generated in the 'xtal' folder. An example for fcc aluminum is shown below.

```
crystal system ---> 1
a [nm] = 0.405
Enter space group number : 225
Atomic number : 13
Fractional coordinates etc. : 0.0,0.0,0.0,1.0,0.00746
Another atom ? (y/n)  n
Enter output file name : Al.xtal
```

**DO NOT USE SPACES IN ANY OF YOUR ENTRIES.**

To confirm that the crystal data was read in properly, make sure you see this in the printed output:

```
 ->  Atomic number : 40
->  Fractional coordinates, site occupation, and Debye-Waller Factor [nm^2] : 0,0,0,0.85,0.0052
   ->  0.0000000   0.0000000   0.0000000   0.8500000   0.0052000
```

Not this:

```
 ->  Atomic number : 40
->  Fractional coordinates, site occupation, and Debye-Waller Factor [nm^2] : 0.0, 0.0, 0.0, 0.85, 0
.0052
   ->  0.0000000  **********  **********  **********  **********
```

Isotropic Debye-Waller factor is in units of nm^2. If you don't know, you can make up a reasonable value (0.004-0.006). A list of Debye-Waller factors for pure elements can be found in: L.-M. Peng, G. Ren, S.L. Dudarev, and M.J. Whelan. *Debye–Waller Factors and Absorptive Scattering Factors of Elemental Crystals*. Acta Crystall. A, **52**:456–470, 1996.

Note: If your atomic coordinates are at a high symmetry position that are not a nice number (e.g. 1/3 for hexagonal crystal system), you should instead run EMmkxtal using the following command to use Wyckoff mode:

```
eddie@X22:~/EMsoftfiles/EMData/191013_Ti_hcp_20kV_master$ EMmkxtal -w
```

**ii. Monte Carlo + Master pattern simulation**

Follow the instructions here to perform the Monte Carlo simulations and master pattern simulations: https://github.com/EMsoft-org/EMsoft/wiki/EBSD-Example

## B. CONVERT PATTERNS TO 8BIT AND STORE IN BINARY FORMAT

*In this section, you will convert the images into 8bit images (if necessary) and store them in a single .data file that EMsoft can read.*

1. In MATLAB, open the script *ConvertStorePatternsAsBinary.m*. You will see a block of code at the top labeled 'INPUT PARAMETERS'. Fill in the parameters.

- Note that **'outputfolder' must be different from 'inputfolder'**, as the program saves the padded images with the same name but in this new location.

2. Run the script. This will take a few minutes. Once the script has finished running, you will find see all of the converted images in the location specified by 'outputfolder'. You will also find the .data binary file containing all of the patterns in the location specified by 'dataname'.

# C. EXTRACT PATTERNS AND RELEVANT INFO

*During this step, you will extract 10 good patterns from your dataset that will be used later for checking the master pattern and fitting the pattern center. You will also extract the orientations of these patterns and the Hough pattern center.*

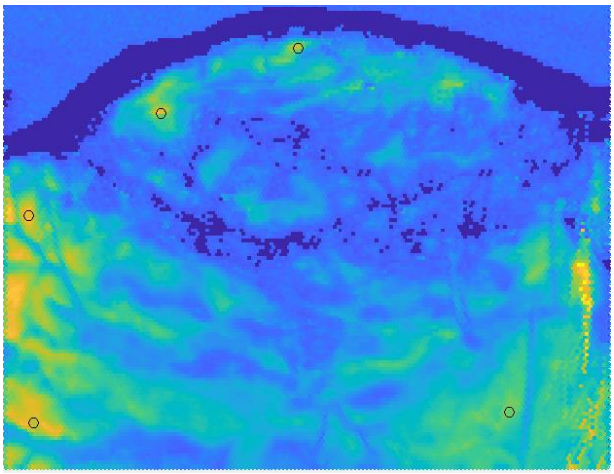
### i. Pick 10 good patterns

*In this step, we will pick 10 good patterns to fit the pattern center with.*

1. Open the *FindMapPoints_edaxang.m* script in MATLAB.

2. Fill in the parameters, and run the script (will take a few minutes). We recommend plotting IQ.

3. Once the plot appears, click 10 points with high IQ (yellow). If possible, try to pick points from all locations around the map and in different grains. You can do more or less than 10 if you want--more patterns give a more accurate pattern center but takes more time.



4. Some info will also appear in the MATLAB terminal for each point you clicked. Copy this information into a .txt file so you have it for future reference.

| index: | x, | y. | phi1, | PHI, | phi2 |
|---|---|---|---|---|---|
| 1991: | 5.7750, | 0.7794. | 112.2613, | 34.9882, | 115.5003 |
| 4986: | 3.1125, | 2.0135. | 7.8770, | 98.6421, | 217.8133 |
| 9736: | 0.4875, | 3.9621. | 76.5747, | 75.8951, | 38.1962 |
| 19148: | 0.6000, | 7.7942. | 216.1294, | 143.1329, | 347.1511 |
| 18794: | 9.9375, | 7.5994. | 328.3444, | 63.4041, | 255.3633 |

5. Copy these images (which are labeled by the index shown above) into a folder within your EMData folder that can be easily accessed later (where you want to store your indexed data).

**ii. Getting the Hough pattern center**

*Now, you will locate the pattern center used by the microscope Hough indexing.*

1. Open the MATLAB script *GetPatternCenter_edaxang.m*.

2. Fill in the input parameters and run.

3. The pattern center in EMsoft coordinates will be displayed.

```
Pattern center (EMsoft coordinates):
  xpc = 3.3704 px
  ypc = 56.6829 px
  L = 2546.93 um
```

**Note that this script converts the pattern center from the typical fraction detector width ($X^*$, $Y^*$, $Z^*$) to EMsoft units (xpc in px, ypc in px, L in microns). The conversions (from EDAX convention, note that Oxford and Bruker have different conventions) are as follows:*

$$xpc = numsx * (X^* - 0.5)$$

$$ypc = numsy * (Y^* - 0.5)$$

$$L = Z^* * numsx * delta$$

## D. SIMULATE EBSD PATTERNS

**In this step, we will simulate a pattern and compare it to the experimental pattern to check that the master pattern is ok and that the Hough orientations and pattern center are reasonable starting points for fitting the pattern center.*

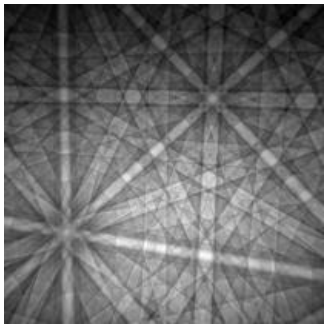
1. In MATLAB, open *the RunEMEBSD.m script.*

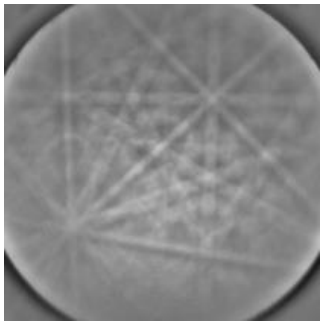
2. Fill in the parameters. Enter the Euler angles for the patterns selected in Step C.i. Fill in the pattern center you determined above in Step C.ii.

3. Run the script. The images will be saved in the location specified.

4. In MATLAB, open the ComparePatterns.*m* script. For each pattern, enter the paths to the simulated and experimental patterns, and run the script. It will output an intensity difference plot as well as another window that flashes between the two patterns.

5. If the patterns look basically the same such as below, then everything is working properly, and you can continue. If not, there is something wrong...





## E. FITTING THE PATTERN CENTER

*To successfully perform a dictionary indexing run, the pattern center must be known to a higher degree of accuracy than given in the Hough data off the microscope (determined in Step C.ii). This section will walk through how to perform this fitting using the pcglobal package.*

**You can also use other software to fit the pattern center, such as EMsoft's EFit or EMDPFit programs, but pcglobal gives better accuracy.*

1. Navigate to the location of your pcglobal directory. In MATLAB, open the script *RunPCfit_loop.m*.

2. Fill in the input parameters, and run the script. This will take some time (~7 min/pattern on our 4-core Intel i7-3770K CPU and an NVIDIA GeForce GTX 650 Ti GPU).

3. Once completed, accurate pattern center values that can be used for dictionary indexing will be printed to the screen (and saved to a .txt file).

```
Fitted pattern center (average of 5 patterns):
  xpc = 9.7354 (X* = 0.523402)
  ypc = 43.0779 (Y* = 0.603553)
  L = 2510.68 (Z* = 0.706836)
```

**If you see that the program has printed any warning messages such as these,*

```
WARNING: L is near search edge. trust_L = 500.00, delta_L = 500.00.
WARNING: ypc is near search edge. trust_ypc = 5.0000, delta_ypc = 5.0000.
WARNING: euler is near search edge.
```

*rerun the RunPCfit_loop.m program with increased trust radius parameters. Also adjust the starting L, xpc, and ypc values to match the outputted average pattern center. And edit the starting euler angles to match the outputted euler angles.*

## F. INDEXING THE DATASET

*This section will detail dictionary indexing+refinement in a single step, using EMsoft. This first indexes the data using a discrete grid of orientations (usually to within ~0.8deg) using the EMEBSDDI program, and then it goes back through the data and optimizes the orientation at every map point to <0.2deg accuracy using the EMFitOrientation program.*

*-You can also only run the dictionary indexing program if you are happy with a discretely indexed orientation. In this case, use the RunEMEBSDDI.m program.*

*-You can separately run the RunEMEBSDDI.m program for dictionary indexing and the RunEMFitOrientation.m program for refinement if you want.*

*-You can also use the EBSDrefine package (https://github.com/epang22/EBSDrefine), which in many cases is faster and more accurate than EMFitOrientation (especially for resolving pseudosymmetry).*

1. In MATLAB, open the script *RunEMEBSDDI_refine.m*.

2. Fill in the parameters.

- Use the fitted pattern center from Step E
- Standard value for `N = 90` (see this paper for more information: S Singh and M De Graef 2016 *Modelling Simul. Mater. Sci. Eng.* **24** 085013)

3. Run the script. This will take some time (~2.5 h using default parameters on an fcc material on our 4-core Intel i7-3770K CPU and an NVIDIA GeForce GTX 650 Ti GPU). The script will generate a bunch of files. **Your final refined data is contained in *[data.outputname]_EMFitOrientation.ang*.** This file can be read by MTEX or OIM Analysis for plotting.