EMSOFT installation and configuration – Windows
Running EMSOFT independently
More instructions and documentation is available on the EMsoft EBSD Example on GitHub: https://github.com/EMsoft-org/EMsoft/wiki/EBSD-Example

1. Download latest date: EMsoft OSX build from http://www.bluequartz.net/binaries/EMsoft/experimental/
2. Right click on folder and select 'Extract All' (you can save the folder anywhere you want)
3. Copy file named 'tbb.dll' into folder named 'bin'
4. Run 'Emsoftinit.exe'
    1. Right click on this file, select 'Run as Administrator'
    2. In the popup dialog, select 'Read More' (at the top of the dialog box)
    3. Select 'Run anyway' at the bottom of the dialog box
    4. If a popup asks if you would like to allow the program to make changes to the hard drive, select 'yes'
    5. Complete the prompts in the Command Prompt
5. Go to C:\Users\[YOUR USER NAME]\.config\EMsoft
6. Edit the 'EMsoftConfig.json' file
    1. Right click on the .json file and select 'Open with'
    2. Choose a text editor (like Notepad++) or an IDE (like Visual Studio Code)
    3. The file will be partially completed. Delete everything in it
    4. Copy and paste the following code into the .json file:

```
{
        "EMsoftpathname": "C:/Users/[YOUR USER NAME]/['bin' FOLDER FILE PATH]",
        "EMXtalFolderpathname": C:/Users/[YOUR USER NAME]/['bin' FOLDER FILE PATH]",
        "EMdatapathname": "C:/Users/[YOUR USER NAME]/['bin' FOLDER FILE PATH]",
        "EMtmppathname": "C:/Users/[YOUR USER NAME]/.config/EMsoft/tmp/",
        "EMsoftLibraryLocation": "C:/Users/[YOUR USER NAME]/['bin' FOLDER FILE PATH]",
        "EMNotify": "No",
        "Release": "No",
        "Develop": "No",
        "UserName": "[YOUR USER IDENTIFIER]",
        "UserEmail": "[YOUR EMAIL]",
        "UserLocation": "[YOUR LOCATION]"
}
```

5. Every time [YOUR USER NAME] is present, replace it with your computer username. Example: [YOUR USER NAME] → bcsyphus
6. Every time [‘bin’ FOLDER PATH NAME] is present, replace it with the path name of the ‘bin’ folder inside the EMsoft folder. MAKE SURE TO USE FORWARD SLASHES. Include ‘bin’ in the file path and leave the final forward slash. Example: [‘bin’ FOLDER PATH NAME] → Documents/GitHub/EMsoft/bin/
7. Every time [YOUR USER IDENTIFIER] is present, replace it with your desired username. Example: [YOUR USER IDENTIFIER] → bsyphus
8. Every time [YOUR EMAIL] is present, replace it with your desired email. Example: [YOUR EMAIL] → bsyphus@byu.edu
9. Every time [YOUR LOCATION] is present, replace it with your desired location. Example: [YOUR LOCATION] → Brigham Young University
10. Do not add extra spaces or punctuation. Do not delete punctuation or formatting from the code provided in these instructions.
11. COMMON ERRORS:
    1. Using back slashes instead of forward slashes
    2. Forgetting/deleting quotation marks, commas, or other punctuation
    3. Adding spaces or extra slashes or punctuation
    4. Adding extra lines before or after the code
    5. Incorrect capitalization
    6. Forgetting the final slash in the EMdataPath or EMsoftPath fields
12. Save and close the .json file

7. Create the .xtal material file (unless you already have xtal files. Then, just move pre-existing .xtal files into the folder you specified in [‘bin’ FILE PATH NAME], and skip to step 8).
    1. In the Command Prompt, navigate to the folder specified in [‘bin’ FILE PATH NAME] by entering the following command and replacing [‘bin’ FILE PATH NAME] in the command as instructed above, but YOU MUST USE BACK SLASHES THIS TIME
       cd [‘bin’ FILE PATH NAME]
    2. Enter the following command into the Command Prompt to launch the .xtal file generator:
       EMmkxtal
    3. Follow the prompts and input all of the crystal structure information
    4. Follow this pattern for every .xtal file: save the file as ‘[MATERIAL NAME].xtal’. Example: [MATERIAL NAME] → ferrite
    5. Pro tip: you can see the list of usable material names in the Main GUI of OpenXY. YOU MUST MATCH ONE OF THESE OPTIONS.
8. Create the first .template file for the first .nml file using the Command Prompt

1. Enter the following command into the Command Prompt to create the template file
   EMMCOpenCL -t
2. In the file explorer GUI, navigate to the ‘bin’ folder and check that a new file named ‘EMMCOpenCL.template’ was created
3. If there is no file by that name, you can copy the ‘EMMCOpenCL.template’ file from the ‘Namelist Templates’ folder (a folder inside the ‘bin’ folder) into the ‘bin’ folder.
    1. DO NOT use the old templates in the ‘examples’ folder

9. Rename ‘EMMCOpenCL.template’ in the ‘bin’ folder to ‘[MATERIAL NAME]_EMMC.nml’. Replace [MATERIAL NAME] as directed above.
    1. If there is a warning popup asking if you are sure you want to change the file name extension, select ‘yes’
10. Open your newly renamed .nml file in a text editor or IDE.
11. Change line 5 from [xtalname = ‘undefined’] to xtalname = ‘[XTAL FILE]’. Replace [XTAL FILE] with the name of the xtal file you created earlier.
12. Pro tip: Reduce the number of electrons (line 51, totnum_el) if you want the code to run faster.
13. Change line 74 from [dataname = ‘MCoutput.h5’] to dataname = ‘[H5 NAME]’ and replace [H5 NAME] with ‘MCoutput_[MATERIAL NAME].nml’. Replace [MATERIAL NAME] as directed above.
14. Adjust other settings if desired. Save and close the .nml file.
15. Run the following command in the Command Prompt to create the .h5 Monte Carlo file. Replace [NML FILE NAME] with the name of the .nml you just created. (default output file name will be ‘MCoutput.h5’ and it will save to the EMdata folder)
    EMMCOpenCL [NML FILE NAME].nml
16. This produces lots of output – see https://github.com/EMsoft-org/EMsoft/wiki/EBSD-Example to compare outputs
17. Check in the ‘bin’ folder for the .h5 file
18. In the File Explorer GUI, copy the ‘BetheParameters.template’ file from ‘Namelist Templates’ to ‘bin’
19. Rename ‘BetheParameters.template’ to ‘BetheParameters.nml’
20. Copy ‘EMEBSDmaster.template’ to ‘bin’ from ‘Namelist templates’
21. Rename ‘EMEBSDmaster.template’ to ‘[MATERIAL NAME]_EMEBSDmaster.nml’
22. Open the ‘[MATERIAL NAME]_EMEBSDmaster.nml’ file in a text editor or IDE
23. Change line 15 from [energyfile = ‘MCoutput.h5’] to energyfile = ‘[H5 NAME]’
24. Other parameters are editable, but the defaults are sufficient. Save and close ‘[MATERIAL NAME]_EMEBSDmaster.nml’

25. Run the following command in the Command Prompt to execute the EMEBSDmaster file
    EMEBSDmaster [MATERIAL NAME]_EMEBSDmaster.nml
26. There will be a lot of output. Compare output at https://github.com/EMsoft-org/EMsoft/wiki/EBSD-Example
27. Copy 'EMEBSD.template' from the 'Namelist Template' folder to the 'bin' folder
28. Rename 'EMEBSD.template' to 'EMEBSD_[MATERIAL NAME].nml'
29. Open the 'EMEBSD_[MATERIAL NAME].nml' file in a text editor or IDE
30. Change line 11 from [numsx = 0,] to numsx = 640,
31. Change line 12 from [numsy = 0,] to numsy = 480,
32. Change line 34 from [masterfile = 'MCouput.h5'] to masterfile = '[H5 NAME]'
33. Save and close 'EMEBSD_[MATERIAL NAME].nml' file
34. Create a new text file in a text editor or IDE. Name it 'testeuler.txt' and save it to ['bin' FOLDER PATH NAME]
    1. Copy and paste the below text into the text file:

       eu
       2
       0.0, 0.0, 0.0
       120.0, 45.0, 60.0

    2. See https://github.com/EMsoft-org/EMsoft/wiki/EBSD-Example for an explanation of this text file
    3. Save and close the 'testeuler.txt' file
35. Run the following command in the Command Prompt to execute the EMEBSD file
    EMEBSD EMEBSD_[MATERIAL NAME].nml
36. Again, lots of outputs. Once the program is finished, an HDF5 file should be present in your ['bin' FOLDER PATH NAME] folder
37. Copy seven files from the 'bin' folder into another folder to keep organization. If you wish to run EMSoft on the same data again in the future, make sure to copy these files back into the folder, and only do step 35. See below list of files to remove from the 'bin' folder:
    BetheParamters.nml
    EMEBSD_[MATERIAL NAME].nml
    [MATERIAL NAME]_EMEBSDmaster.nml
    [MATERIAL NAME]_EMMC.nml
    [H5 NAME].h5
    testeuler.txt
    [MATERIAL NAME].xtal

Running EMSOFT with OpenXY

1. Run all steps above exactly as written, except step 37.
2. Open the OpenXY GUI.
3. Select all scan files, etc. as normal.
4. Select the material from the drop down that matches the naming convention you used above.
5. Select ‘Advanced Settings’ in the top left corner.
6. Select ‘Simulated Dynamic”
7. Select folder containing the .json file
8. Select Calculation method
9. Run
10. Do step 37 if desired.