Presentation on how to install LAUETOOLSNN

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[1]French CRG beamline BM32, ESRF, Grenoble

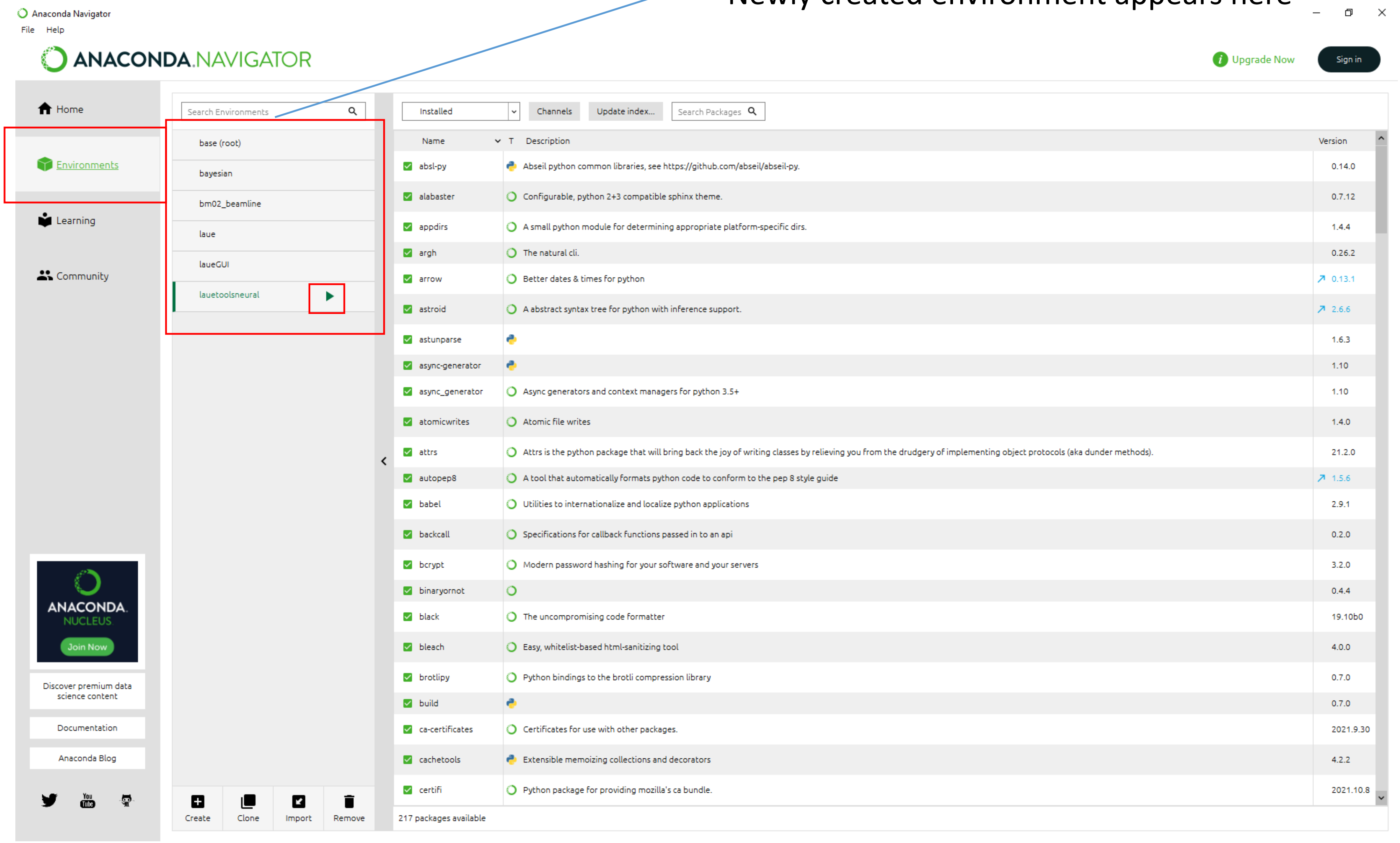
Requirements

- Anaconda distribution
  - https://www.anaconda.com/products/individual

- Create a new environment
  - conda create –name lauenn python=3.8
  - Lauetoolsnn requires python >3.6

- Activate the created environment and install lauetoolsnn
  - conda activate lauenn
  - pip install lauetoolsnn
    - Includes all required libraries (in case of errors; try the last command with “--user” suffix)

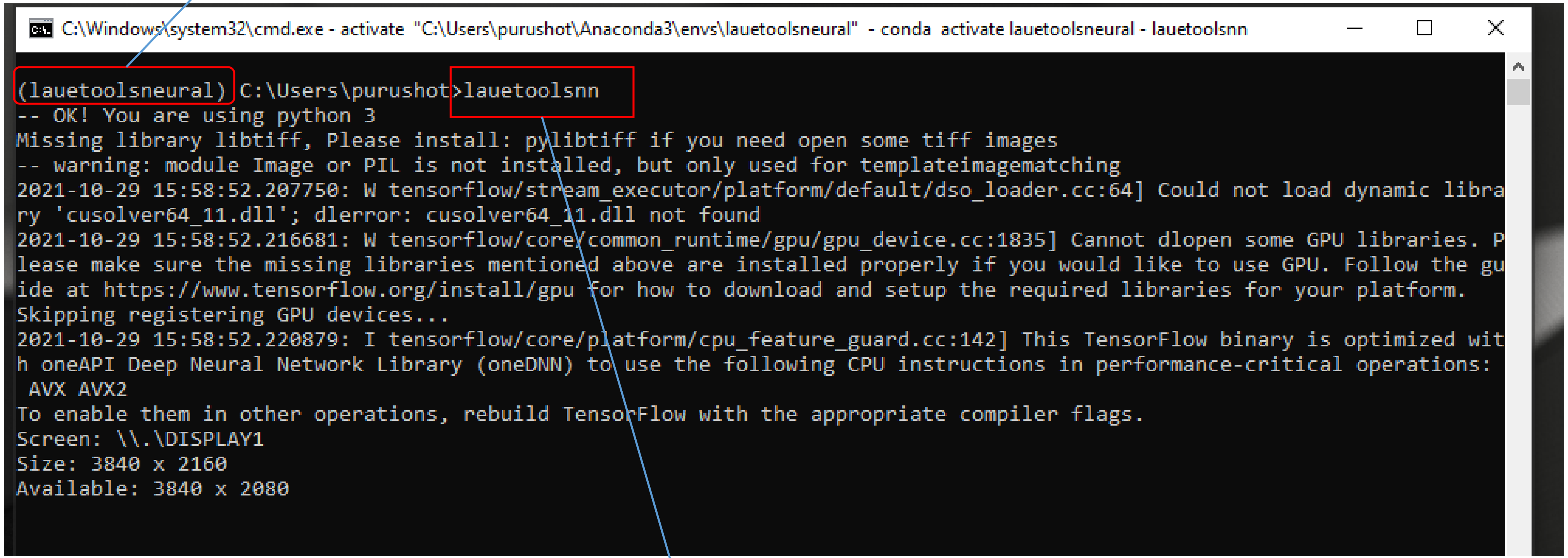
Newly created environment appears here



	Name	T	Description	Version
☑	absl-py		Abseil python common libraries, see https://github.com/abseil/abseil-py.	0.14.0
☑	alabaster	○	Configurable, python 2+3 compatible sphinx theme.	0.7.12
☑	appdirs	○	A small python module for determining appropriate platform-specific dirs.	1.4.4
☑	argh	○	The natural cli.	0.26.2
☑	arrow	○	Better dates & times for python	↗ 0.13.1
☑	astroid	○	A abstract syntax tree for python with inference support.	↗ 2.6.6
☑	astunparse			1.6.3
☑	async-generator			1.10
☑	async_generator	○	Async generators and context managers for python 3.5+	1.10
☑	atomicwrites	○	Atomic file writes	1.4.0
☑	attrs	○	Attrs is the python package that will bring back the joy of writing classes by relieving you from the drudgery of implementing object protocols (aka dunder methods).	21.2.0
☑	autopep8	○	A tool that automatically formats python code to conform to the pep 8 style guide	↗ 1.5.6
☑	babel	○	Utilities to internationalize and localize python applications	2.9.1
☑	backcall	○	Specifications for callback functions passed in to an api	0.2.0
☑	bcrypt	○	Modern password hashing for your software and your servers	3.2.0
☑	binaryornot	○		0.4.4
☑	black	○	The uncompromising code formatter	19.10b0
☑	bleach	○	Easy, whitelist-based html-sanitizing tool	4.0.0
☑	brotlipy	○	Python bindings to the brotli compression library	0.7.0
☑	build			0.7.0
☑	ca-certificates	○	Certificates for use with other packages.	2021.9.30
☑	cachetools		Extensible memoizing collections and decorators	4.2.2
☑	certifi	○	Python package for providing mozilla's ca bundle.	2021.10.8

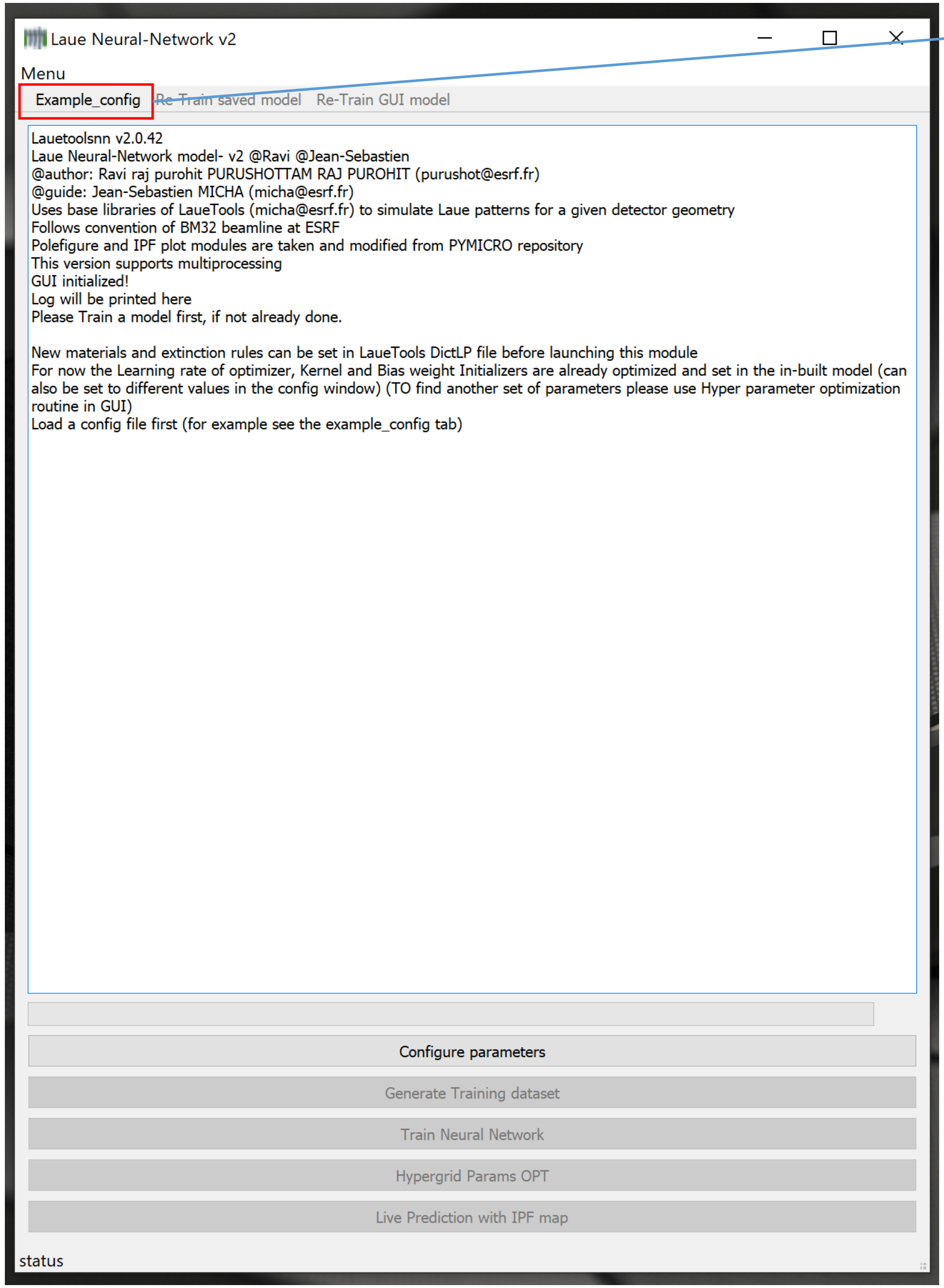
217 packages available

Conda environment with lauetoolsnn installed


C:\Windows\system32\cmd.exe - activate "C:\Users\purushot\Anaconda3\envs\lauetoolsneural" - conda activate lauetoolsneural - lauetoolsnn

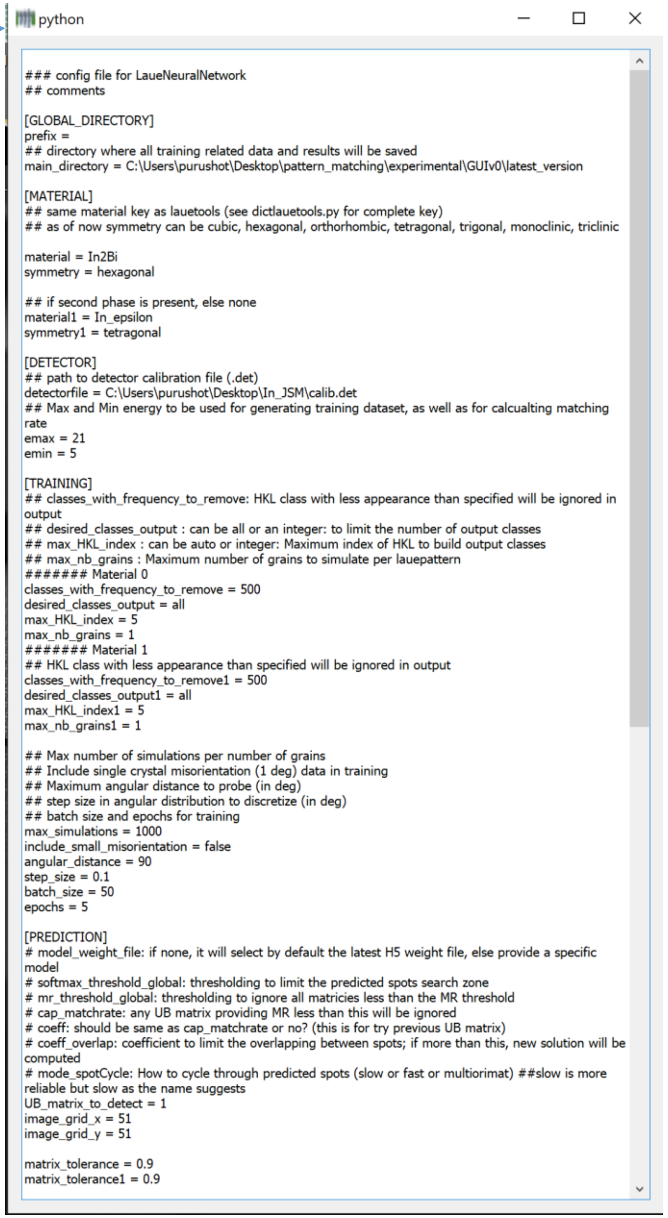
```
(lauetoolsneural) C:\Users\purushot>lauetoolsnn
-- OK! You are using python 3
Missing library libtiff, Please install: pylibtiff if you need open some tiff images
-- warning: module Image or PIL is not installed, but only used for templateimagematching
2021-10-29 15:58:52.207750: W tensorflow/stream_executor/platform/default/dso_loader.cc:64] Could not load dynamic libra
ry 'cusolver64_11.dll'; dlerror: cusolver64_11.dll not found
2021-10-29 15:58:52.216681: W tensorflow/core/common_runtime/gpu/gpu_device.cc:1835] Cannot dlopen some GPU libraries. P
lease make sure the missing libraries mentioned above are installed properly if you would like to use GPU. Follow the gu
ide at https://www.tensorflow.org/install/gpu for how to download and setup the required libraries for your platform.
Skipping registering GPU devices...
2021-10-29 15:58:52.220879: I tensorflow/core/platform/cpu_feature_guard.cc:142] This TensorFlow binary is optimized wit
h oneAPI Deep Neural Network Library (oneDNN) to use the following CPU instructions in performance-critical operations:
 AVX AVX2
To enable them in other operations, rebuild TensorFlow with the appropriate compiler flags.
Screen: \\.\DISPLAY1
Size: 3840 x 2160
Available: 3840 x 2080
```

Once installed, launch the GUI by calling lauetoolsnn in the terminal



```
Lauetoolsnn v2.0.42
Laue Neural-Network model- v2 @Ravi @Jean-Sebastien
@author: Ravi raj purohit PURUSHOTTAM RAJ PUROHIT (purushot@esrf.fr)
@guide: Jean-Sebastien MICHA (micha@esrf.fr)
Uses base libraries of LaueTools (micha@esrf.fr) to simulate Laue patterns for a given detector geometry
Follows convention of BM32 beamline at ESRF
Polefigure and IPF plot modules are taken and modified from PYMICRO repository
This version supports multiprocessing
GUI initialized!
Log will be printed here
Please Train a model first, if not already done.

New materials and extinction rules can be set in LaueTools DictLP file before launching this module
For now the Learning rate of optimizer, Kernel and Bias weight Initializers are already optimized and set in the in-built model (can
also be set to different values in the config window) (TO find another set of parameters please use Hyper parameter optimization
routine in GUI)
Load a config file first (for example see the example_config tab)
```



```
### config file for LaueNeuralNetwork
## comments

[GLOBAL_DIRECTORY]
prefix =
## directory where all training related data and results will be saved
main_directory = C:\Users\purushot\Desktop\pattern_matching\experimental\GUIv0\latest_version

[MATERIAL]
## same material key as lauetools (see dictlauetools.py for complete key)
## as of now symmetry can be cubic, hexagonal, orthorhombic, tetragonal, trigonal, monoclinic, triclinic

material = In2Bi
symmetry = hexagonal

## if second phase is present, else none
material1 = In_epsilon
symmetry1 = tetragonal

[DETECTOR]
## path to detector calibration file (.det)
detectorfile = C:\Users\purushot\Desktop\In_JSM\calib.det
## Max and Min energy to be used for generating training dataset, as well as for calcualting matching
rate
emax = 21
emin = 5

[TRAINING]
## classes_with_frequency_to_remove: HKL class with less appearance than specified will be ignored in
output
## desired_classes_output : can be all or an integer: to limit the number of output classes
## max_HKL_index : can be auto or integer: Maximum index of HKL to build output classes
## max_nb_grains : Maximum number of grains to simulate per lauepattern
####### Material 0
classes_with_frequency_to_remove = 500
desired_classes_output = all
max_HKL_index = 5
max_nb_grains = 1
####### Material 1
## HKL class with less appearance than specified will be ignored in output
classes_with_frequency_to_remove1 = 500
desired_classes_output1 = all
max_HKL_index1 = 5
max_nb_grains1 = 1

## Max number of simulations per number of grains
## Include single crystal misorientation (1 deg) data in training
## Maximum angular distance to probe (in deg)
## step size in angular distribution to discretize (in deg)
## batch size and epochs for training
max_simulations = 1000
include_small_misorientation = false
angular_distance = 90
step_size = 0.1
batch_size = 50
epochs = 5

[PREDICTION]
# model_weight_file: if none, it will select by default the latest H5 weight file, else provide a specific
model
# softmax_threshold_global: thresholding to limit the predicted spots search zone
# mr_threshold_global: thresholding to ignore all matricies less than the MR threshold
# cap_matchrate: any UB matrix providing MR less than this will be ignored
# coeff: should be same as cap_matchrate or no? (this is for try previous UB matrix)
# coeff_overlap: coefficient to limit the overlapping between spots; if more than this, new solution will be
computed
# mode_spotCycle: How to cycle through predicted spots (slow or fast or multiorimat) ##slow is more
reliable but slow as the name suggests
UB_matrix_to_detect = 1
image_grid_x = 51
image_grid_y = 51

matrix_tolerance = 0.9
matrix_tolerance1 = 0.9
```

Example_config: provides a template to create a config file for automated analysis

Setting in config file

```
### config file for LaueNeuralNetwork

[GLOBAL_DIRECTORY]
prefix =
## directory where all training related data and results will be saved
main_directory = C:\Users\purushot\Desktop\pattern_matching\experimental\GUIv0\latest_version

```

Prefix: specify a string to distinguish the model files or keep blank

```
[MATERIAL]
## same material key as lauetools (see dictlauetools.py for complete key)
## as of now symmetry can be cubic, hexagonal, orthorhombic, tetragonal, trigonal, monoclinic, triclinic

material = In2Bi
symmetry = hexagonal


## if second phase is present, else none
material1 = In_epsilon
symmetry1 = tetragonal

```

If 2 materials present specify them here; in case of only 1 material, keep none for the other

```
[DETECTOR]
## path to detector calibration file (.det)
detectorfile = C:\Users\purushot\Desktop\In_JSM\calib.det
## Max and Min energy to be used for generating training dataset, as well as for calcualting matching rate
emax = 21
emin = 5

```

Detector settings

Setting in config file

- [TRAINING]
- ## classes_with_frequency_to_remove: HKL class with less appearance than specified will be ignored in output
- ## desired_classes_output : can be all or an integer: to limit the number of output classes
- ## max_HKL_index : can be auto or integer: Maximum index of HKL to build output classes
- ## max_nb_grains : Maximum number of grains to simulate per lauepattern
- ####### Material 0
- classes_with_frequency_to_remove = 500
- desired_classes_output = all
- max_HKL_index = 5
- max_nb_grains = 1
- ####### Material 1
- ## HKL class with less appearance than specified will be ignored in output
- classes_with_frequency_to_remove1 = 500
- desired_classes_output1 = all
- max_HKL_index1 = 5
- max_nb_grains1 = 1
-
- ## Max number of simulations per number of grains
- ## Include single crystal misorientation (1 deg) data in training
- ## Maximum angular distance to probe (in deg)
- ## step size in angular distribution to discretize (in deg)
- ## batch size and epochs for training
- max_simulations = 1000
- include_small_misorientation = false
- angular_distance = 90
- step_size = 0.1
- batch_size = 50
- epochs = 5
-

Settings related to Training of Neural network

If unsure, just modify max_nb_grains and max_nb_grains1 ; i.e. maximum grains expected per material

All the other settings can be kept same

Setting in config file

- [PREDICTION]
- # model_weight_file: if none, it will select by default the latest H5 weight file, else provide a specific model
- # softmax_threshold_global: thresholding to limit the predicted spots search zone
- # mr_threshold_global: thresholding to ignore all matricies less than the MR threshold
- # cap_matchrate: any UB matrix providing MR less than this will be ignored
- # coeff: should be same as cap_matchrate or no? (this is for try previous UB matrix)
- # coeff_overlap: coefficient to limit the overlapping between spots; if more than this, new solution will be computed
- # mode_spotCycle: How to cycle through predicted spots (slow or fast or multiorimat) ##slow is more reliable but slow as the name suggests
- UB_matrix_to_detect = 1
- image_grid_x = 51
- image_grid_y = 51
- matrix_tolerance = 0.9
- matrix_tolerance1 = 0.9
- material0_limit = 1
- material1_limit = 1
- model_weight_file = none
- softmax_threshold_global = 0.85
- mr_threshold_global = 0.80
- cap_matchrate = 0.01
- coeff = 0.3
- coeff_overlap = 0.3
- mode_spotCycle = slow
- ##true for few crystal and prefered texture case, otherwise time consuming; advised for single phase alone
- use_previous = true

Settings related to Prediction

if unsure, just modify
Grid_x and grid_y : dimension (steps) of scan area

matrix_tolerance and matrix_tolerance1 ; tolerance angle to search for spots: keep 0.5 if unsure

How many grains to detect per material: material0_limit, material1_limit restricts that
use_previous = true; for trying previously identified rotation matrix

mode_spotCycle: graphmode, beamtime mode are the fastest; subsequently on can use also slow mode for more thorough search.

All the other settings can be kept same

Setting in config file

- [EXPERIMENT]
- experiment_directory = C:\Users\purushot\Desktop\In_JSM\ech875_ROI01
- experiment_file_prefix = ech875_ROI01_
- [PEAKSEARCH]
- intensity_threshold = 90
- boxsize = 15
- fit_peaks_gaussian = 1
- FitPixelDev = 15
- NumberMaxofFits = 3000

- [STRAINCALCULATION]
- strain_compute = true
- tolerance_strain_refinement = 0.7,0.6,0.5,0.4,0.3,0.2
- tolerance_strain_refinement1 = 0.7,0.6,0.5,0.4,0.3,0.2

- [POSTPROCESS]
- hkls_subsets = [1,1,0],[1,0,0],[1,1,1]
- [DEVELOPMENT]
- # could be 1 or 2 / none in case of single phase
- material_phase_always_present = 1
- write_MTEX_file = true
- material0_lauegroup = 9
- material1_lauegroup = 5

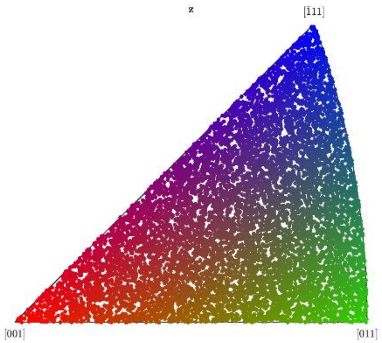
Settings related to Experiment and misc

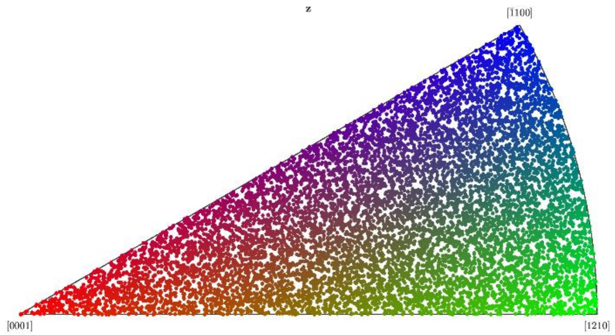
material_phase_always_present = 1; forces the neural network to predict always the first grain from material 1; leads to nice plots

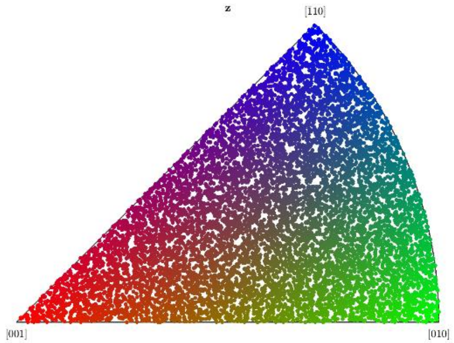
MTEX output for plotting PF and IPFs ; specifiy the proper laue group to get proper colors

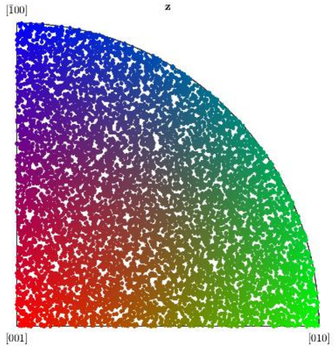
Predefined uniform orientation distribution for all symmetries (used during training)

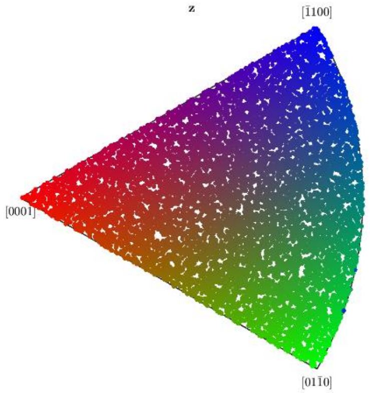
- It is possible to define particular orientations too (in case of preferred texture) → however this will lead to bias in model


z
$[\bar{1}11]$
[001]
[011]


z
$[\bar{1}100]$
[0001]
[1210]


z
$[\bar{1}10]$
[001]
[010]


$[\bar{1}00]$
z
[001]
[010]


z
$[\bar{1}100]$
$[000\bar{1}]$
$[01\bar{1}0]$