User Guide For ROME2D

Intel Parallel Computing Center For Structural Biology

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1.Install

1) make sure you have install intel complier,intel mkl library and intel mpi library.
2) If you not install mpi library,please change:
   ```
   CC := mpiicpc to CC := icpc
   LD := mpiicpc to LD := icpc
   MACROS := -DUSEMPI -DCOMMANDLINE to MACROS := -DCOMMANDLINE
   ```
   in Makefile.
3) build for ML2D:
   make
   make rome_ml2d
4) build for GTM:
   offload code(by default):
   make
   make rome_gtm
   no-offload code:
   export export OFFLOAD="-qno-offload”
   make
   make rome_gtm
5) the binary file will be located at bin folder in current dictionary.

2.ML2D Usage

Basic usage

We use the ML2D to find the orientation of all images(or particles),you need prepare all *.mrcs file and one *.star file,put them on same dictionary,this is the command to run rome_ml2d:

./bin/rome_gtm –i star_file_name –o output_file_name –n number_of images(or particle) -k number_of_classes_you_want_to_classification –iter number_of_iterations –pixel pixel_size

the output file will be a new *.star file(this is needed for next GTM step) with right orientation and the classaverage mrcs file.you can find more example how to use this at scripts floder or 4.Example chapter.

Some additional options

- The 2D search offset_range is -10~10,offset_step is 2 and rotation step is 10 by default,many times this work well,you can set these parameters by using -offset_range,-offset_step and –offset_step options.
- The ML2D algorithm uses the average image as classaverage template,so using what image as classaverage template is important,how to order images may get different result,you can set the –random_seed to see this.
- -pool option means how many images process each time,this should fit memory size,the appropriate pool may increase the performace.

3.GTM Usage

Basic usage

After finding all images(or particles)' orientation with rome_ml2d,you get a new *.star file from rome_ml2d.take that star file as input star file for rom_gtm and prepare to classify the images data by GTM,the basic usage of GTM is:

./bin/rome_gtm –i star_file_name –o output_file_name –n number_of images(or particle) -k number_of_classes_you_want_to_classification –iter number_of_iterations –pixel pixel_size

you can find more example how to use this at scripts floder or 4.Example chapter.

Some advanced option

- By default,the alpha value in GTM is not updated and the beta value in GTM is updated,we find this setting can get good result,but you can change this setting by –updateAlpha(0 or 1) and –updateBeta(0 or 1).
- We donnot find some good solution for the convergence condition of GTM algorithm,so donnot set –precision(default is 10e-12) so large,using the default setting is best.
- The gtm algorithm is implemented on XeonPhi,if you have install XeonPhi on your cluster,you can build the code for offload mode.but we cannot guarantee the XeonPhi can accelerate your this code,if your dataset is so small,do not using offload,or set the –nummic(the number of mic coard) to 0.if you using the XeonPhi,the work load put to XeonPhi will be determined by some heuristic method,you can also set how much work put th XeonPhi by hand,just setting –loadmic(0~1).

4.ROME2D GUI

The ROME2D GUI is coded by python which is located at scripts folder,for using this,first you should install python in your computer,than using **python rome_dict/script/rome_viewer.py** to open the GUI.You can open the *.star file(for particle picking) or *.mrcs file(for generate image view).you can find more detail about how to use this GUI picking particle in chapter5 Example.

5.Example

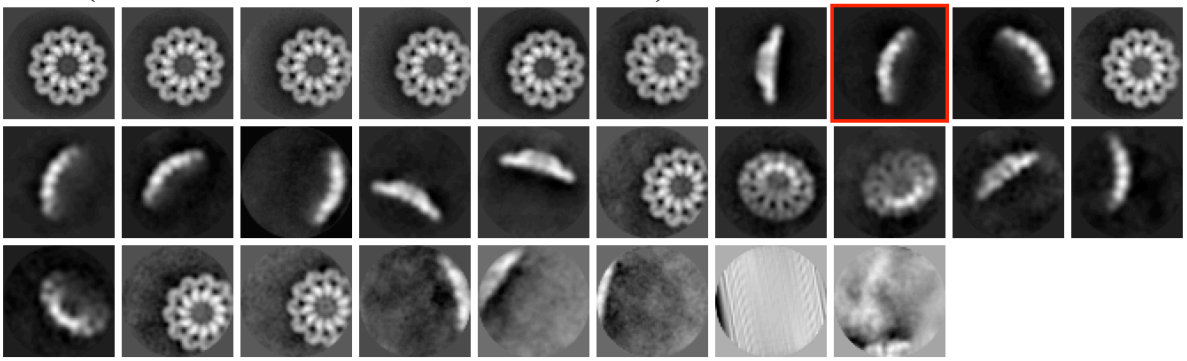
The data classification step

1) run the ml2d to find the orientation of data.
2) view the result get by ML2D,decided how to use GTM,we can process all image together (dataset:BC,fc) or select specific class then run the gtm(dataset:Inf)
3) run the GTM to find the conformation of the data.

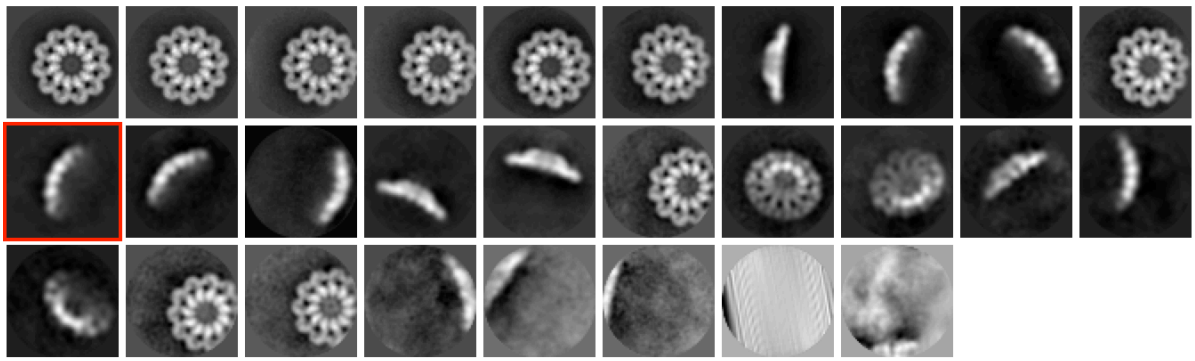
Example 1: inflammasome

script file:script/runInf.sh

1) run the ML2D to find the orientation of the Inf dataset,open the 50th iterations' *.star file(make sure _iter50.star and _iter50.mrcs in same directionary).select the class8 and class45 respectively and save them(file-save selected class's star file)

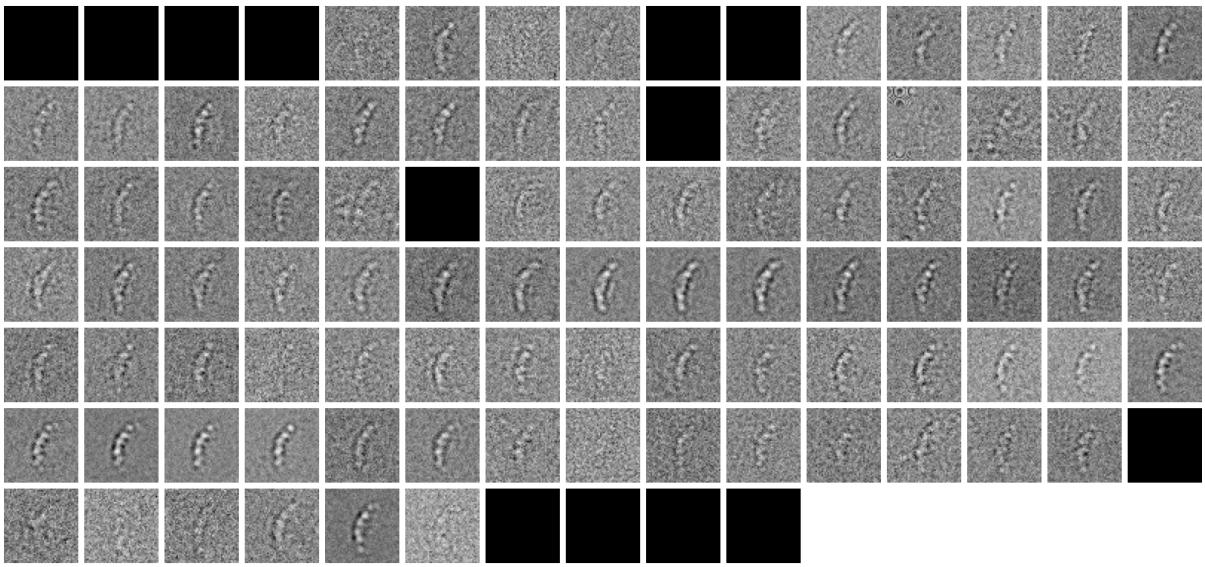


select the 8th image(class).class Info : images = 533,probability = 0.0326873343019

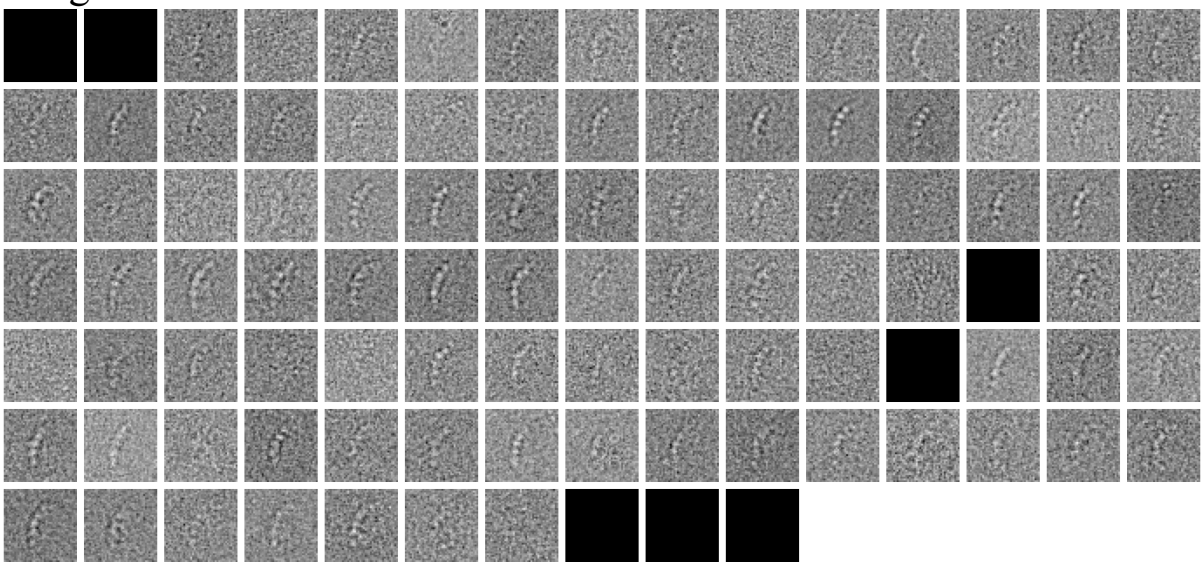


select the 45th image(class).class Info : images = 344,probability = 0.0210965159472

2) run gtm for ml2d class8:



3) run gtm for ml2d class45:



Example 2: BC

script file:script/runBC.sh

Example 3: fc

script file:script/runfc.sh