Summer 2023 Research Journal

08/03/23

ace_amr numpy array in ace_julia is not the same as the one in lagspace. I need to figure out why.

- things to test:
  - make sure averaging is the same
  - check parameters
  - Can we recreate the same numpy array in ace_julia?

This is the script given to me by the organizers of ACE https://github.com/ACEsuit/ACEfit.jl/issues/28

This does an averaging.

Fixed Length Methods

- PDF
- Kmeans
  - both with and without PCA
  - both Kernel and non-kernel PCA
- CUR
- LDF

Hyperparameter Tuning

- Preprocessing data
- grid search

08/02/23

- [ ] get bounding box size for each bacteria and append to csv.
- [ ] get under 20G of data for as many species as possible.
- [ ] upload data to kaggle and add important information to description.
- [x] 3 hours to writing gbcompare paper. No excuses. Write better goals for writing.
- [x] Run quench scripts with increased size for all sigma 3, see homer chat.

TODO:

- [ ] ML/Descriptor/Fix table for ACE

Rendir Quentas

Writing does not come easily for me. If I am not actively writing on a daily basis the paper become a complex puzzle. Almost like each word is a parameter that needs to be optimized and placed correctly. By doing it before anything else I found that starting is the hard part. Spending time writing makes the puzzle seem doable.

I also forgot to push for Gus, shame on me.

08/01/2023

- [x] 10:30 - 11:00 CFM
- [x] 11:00 - 12:30 Find fixed edge length and range of slices for each bacteria.
- [ ] 12:30 - 5:00 GBC paper

How to use 3dmod on supercomputer with macOS

1. install XQuartz
    - https://www.xquartz.org/
2. login to the supercomputer using -X flag i.e. 'ssh -X username@ssh.rc.byu.edu'
    - -X flag allows you to open graphical applications on the supercomputer
3. open the terminal and allocate time on a job node. i.e. 'salloc --time=2:00:00 --mem=2G --x11'
    - --time is the amount of time you want to allocate
    - --mem is the amount of memory you want to allocate
    - --x11 is to open a graphical session
4. Download the IMOD install bash script here
5. Run the bash script. i.e. 'bash -skip -dir ~/Downloads imod_4.11.24_RHEL7-64_CUDA10.1.sh'
    - -skip keeps the script from editing any user files. you need this because it attempts to edit .profile which you cannot edit.
    - -dir is the directory where you want to install IMOD. You need this because you don't have permission to install it in the default location. /usr/local/
6. run 'source ~/Downloads/IMOD/IMOD-linux.sh' to add IMOD to your path.
7. Now anywhere you can run '3dmod' to open 3dmod.

Reading mod files using imodinfo

```
#!/bin/bash

for modfile in yc*/fm.mod
do
        moddir=$(dirname $modfile)
        imodinfo -a $modfile | grep '^slicerAngle' | awk '{print $(NF-
2)","$(NF-1)","$NF}' > $moddir/contour_fm.csv
done
```

This script will go through all the directories in the current directory and find all the fm.mod files. It will then use imodinfo to read the slicerAngle from the mod file and write it to a csv file in the same directory as the mod file.

SSH config

IF you want to open a software on the supercomputer and have it open on your computer you can use the following ssh config. This will allow you to open 3dmod on the supercomputer and have it open on your computer.

```
Host sc
    Hostname ssh.rc.byu.edu
    User cbo27
    ForwardX11 yes
    ControlMaster auto
    ControlPath ~/.ssh/master-%r@%h:%p.socket
    ControlPersist yes
    ServerAliveInterval 300
```

`ForwardX11 yes` is the important line. This tells ssh to forward the X11 session to your computer. You can then open 3dmod on the supercomputer and it will open on your computer.

You might come across an issue where xQuartz does not open when logging in with host. This might be because the master port at `ControlPath` was not opened with forwarding. To fix this you can run `ssh -O exit -S ~/.ssh/master-%r@%h:%p.socket sc` to close the master port. Then you can run `ssh sc` to open a new master port with forwarding.

NOTE: It is important to close xQuartz after you leave your session

08/01/23 Rendir Quentas

I find myself prioritizing BIG(Biophical Image Group) research over writing the gbcompare paper. Only worked on this from 4-5pm.

Things were kinda slow with finding the fixed edge length and tomogram slices for each bacteria. I decided that the range of slices to be 10 minus the min of the picked slices to 10 plus the max of the picked slices. So the sizes wont be the same for each one so it is going to be up to the user to make it work. As far as a bounding box size, I need to see if they are all the same even across different bacteria species.