**EMDA Tutorial for LMB workshop**

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**Installing EMDA:**

As easy as *pip install emda*

EMDA is written to run in both Python2.7 and Python3. However, it prefers Python3 over Python2.7.

**Running EMDA:**

From command line

>> emda option --arguments

EMDA is a python package and you can import with import emda in your python script.

Today, we will be working on following tasks using EMDA.

Tasks:

1. Real space local correlation
2. Fourier shell correlation
3. Fourier space local correlation
4. Map-model FSC
5. Domain overlay
6. Average map calculation

**Real space correlation**

In this case, we calculate the correlation of densities of two maps. To do this, please download the bundle **https://www.ebi.ac.uk/pdbe/entry/emdb/EMD-9931**

move to working directory and untar it.

Before calculating real space correlation, you can calculate the power spectrum and make sure that maps are not lowpass filtered.

To calculate power spectrum

>> emda power --map half1.mrc and look at the values.

To calculate the real space correlation using EMDA just run

>> emda rcc --h1 half1.mrc –h2 half2.mrc --knl 9

Inspect hfmaps\_3dcc\_smax9.mrc and fullmap\_3dcc\_smax9.mrc

Do you think this correlation is meaningful?

**Fourier space 3D correlation**

>> emda fcc --h1 half1.mrc –h2 half2.mrc --knl 9

Look at fouriercorr3d\_fullmap.mrc

What do you see? Do you see a sphere or distorted sphere in some directions? Can you comment on this?

**Fourier Shell Correlation (FSC) using half data**

>> emda halffsc --h1 half1.mrc –h2 half2.mrc

To get the resolution of the full map (without masking) just run

>> emda resol --h1 half1.mrc --h2 half2.mrc

**Apply b-factor to map**

>> emda bfac --map half1.mrc --bfc 30 --out out

Now you can recalculate fsc using this map vs half2.

**Map-model FSC for Validation**

Try this on your own data and models.

>> emda mapmodelfsc --h1 half1.mrc --h2 half2.mrc --mdf fullmode.pdb

This will output two plots. Look at them and criticize.

**Domain overlay**

Download EMD-9931 and EMD-9934. Then get the domains supplied.

Here we are going to overlay domain A in both maps.

>> emda overlay –map emd-9931-hf1.mrc emd-9934-hf1.mrc –msk 9931-domainA.mrc 9934-domainA.mrc

Keep other values defaults.

This will output static.mrc and fitted.mrc. open then in chimera.

Also look at fsc.eps and see the improvement in fsc after alignment.

**Map average**

Now let’s average domain A in both maps. For this we need both half maps in each set.

>> emda average --map emd\_9931\_half\_map\_1.map emd\_9931\_half\_map\_2.map emd\_9934\_half\_map\_1.map emd\_9934\_half\_map\_2.map --msk 6k7g-9931\_A\_mask.mrc 6k7g-9931\_A\_mask.mrc 6k7i-9934\_A\_mask.mrc 6k7i-9934\_A\_mask.mrc

Open one of the averaged maps and compare that with the deposited map in COOT.

You map play with other options in EMDA