Genarris diverse workflow

1. Make geometry.in of a single molecule. Various options include:

* Obtain a .cif file from CCSD, load into Vesta, delete all atoms not belonging to a single molecule, export data, convert from .xyz to geometry.in format
* Draw the molecule in Chemdraw, get 3d coordinates, convert to geometry.in format

1. Relax the single molecule

* Light PBE+TS settings (see control\_single\_molecule.in)

1. Get a volume estimate

* Use “Structure\_Generation\_Batch” procedure
* Overestimate the volume when setting unit\_cell\_volume\_upper\_bound in the conf file
* Underestimate the volume when setting unit\_cell\_volume in the conf file
* Set number\_of\_structures to about 10
* set processes\_limit to 1 in [ISGEP\_master] and up to the number of structures desired (10 in this case) in [structure\_generation\_batch]
* Allocate processes\_limit number of cores in your submission script with the following command in the submission script:

python /path/to/genarris\_master.py volume\_estimate\_generation.conf

* Relax these 10 structures
* Could use FHI\_Aims\_Scavenge and FHI\_Aims\_Batch\_Run as in the example “relaxation.conf”. Then, inside a submission script:

python /path/to/genarris\_master.py relaxation.conf

* Lowest volume is the estimate to use

1. Prepare a single molecule for harris approximation with Harris\_Single\_Molecule\_Prep

python /path/to/genarris\_master.py molecule\_preparation.conf

1. Generate 5000 structures with Structure\_Generation\_Batch

python /path/to/genarris\_master.py generation.conf (aka structure\_generation.conf)

1. Perform Harris Approximation with Harris\_Approximation\_Batch

python /path/to/genarris\_master.py ha.conf

1. Do RCD\_Vector\_Calculation

python /path/to/genarris\_master.py rcd\_5000.conf

1. Do RCD\_Difference\_Folder\_Inner

python /path/to/genarris\_master.py rcd\_folder\_5000.conf

1. Create rcd difference matrix

python combine.py

1. Do Affinity\_Propogation\_Fixed\_Clusters to create 500 clusters of 10 structures each

python /path/to/genarris\_master.py cluster\_500.conf

1. Repeat last step, changing the preference value/range until 500 are chosen
2. Repeat steps 10 – 14 except this time creating 50 clusters (when you do clustering, uncomment examplar\_output\_folder. This time, these will be the final 50 structures.).
3. Relax these 50 structures with light DFT settings (such as in step 6). This is the initial pool.
4. If you didn’t output relaxed structures as jsons in the last step (but you would like those jsons) you may do the FHI\_Aims\_Extract procedure (see ui.conf in Genarris/examples/fhi\_aims\_extract)

python /path/to/genarris\_master.py ui.conf