Installing Genarris

1. Install Anaconda for python 2.7.
2. Follow the direction at the following website to install pymatgen: http://pymatgen.org/installation.html
3. cd to your installation directory of choice and copy the genarris\_installation\_files folder to this directory
4. Incorporate the following PATH and PYTHONPATH commands into your ~/.bashrc

export PYTHONPATH=$INSTALL\_PATH/aimsutils/ase:$PYTHONPATH

export PATH=$INSTALL\_PATH/aimsutils/ase/tools:$HOME/bin:$PATH

Make sure the following PATH command is incopororated into your ~/.bash\_profile

export PATH=$PATH:$HOME/.local/bin

1. Execute the following commands to install aimsutils and Genarris

cd genarris\_installation\_files

./install\_aimsutils\_and\_Genarris.sh

1. Next steps: Follow the instructions in “Genarris\_diverse\_workflow\_tutorial\_assuming\_already\_installed.docx” (all installation (except for maybe some python packages such as numpy that we assume you can install) should be accounted for by the previous commands), modifying the conf\_files and control files as necessary. Use “Documentation\_for\_users\_genarris.docx” to know what the variables mean and which procedure they belong to as well as what each procedure does.