

Prepare mini-Conda environment and install gaft GA-framework

1. Get Miniconda-installer

<https://conda.io/miniconda.html>

1.2 Execute - installation will create conda-workspace in your home directory

chose name for directory and allow to create PATH variable in .bashrc

1.3 Create environment for project - confirm installation of basic packages

conda create -n <env_name> python

1.4 activate it

source activate <env_name>

1.5 upgrade pip

pip install --upgrade pip

2. Set up channels - execute the commands in given order for correct priorities

conda config --add channels defaults

conda config --add channels bioconda

conda config --add channels conda-forge

3. get openMPI and extract

<https://www.open-mpi.org>

tar -xjf <filename.tar.bz2>

3.1 install

./configure --prefix=\$HOME/<install dir> # and go get a coffee

make # go get another one

make install # you know the drill

3.2 add to PATH in /home/<user>/.bashrc

export PATH="\$HOME/<install dir>/bin:\$PATH"

4. Install mpi4py (make sure that the environment is still active)

pip install mpi4py

5. Install gaft - the installation will actually install mpi4py if not present

pip install gaft

6. Run MPI job in SLURM with 'mpi4py'

Take a look at the accompanying "hello_mpi" example based on:

<https://github.com/chunglabmit/phathom/wiki/Using-mpi4py-on-SLURM>

7. Run GAFT example in SLURM

Take a look at the "gaft_intro" example based on:

<https://github.com/PytLab/gaft>