Instruction: Compile SOAP on Desktops

1 Introduction & Preparation

This instruction is for compiling SOAP on the desktops (Iron, Tin, Lead, Zinc, Titanium) in Marom's group. Before you start reading this instruction, make sure the desktop you are working on has a RedHat operating system, and you are the admin of this desktop, since you will need the `sudo` command in this process. If you don't have that, please email Tim trose@andrew.cmu.edu to get it.
Make sure you have the `epfl.tar.gz` file in your desktop, this is the source code you need for compilation.
If you have any questions/comments/suggestions about this instruction, please do not hesistate to contact me.

2 Instructions for Compilation

2.1 Make a Separate Directory and Untar

In this step you need to make a separate directory to put your SOAP source code and all utilities together. Go to your desired folder and make a new directory. I just make a directory called `SOAP` for this usage.

```
mkdir SOAP
mv epfl.tar.gz SOAP
```

Now untar this tar.gz file and you should see a folder named `epfl` after you run the next command

```
tar -zxvf epfl.tar.gz
```

All source code you need is in `epfl` folder.
There is one more thing to address is in the makefile `make.in`, the `-lmkl` flag in the `LDFLAGS` should be removed because you actually do not need this. `make.in` is located at `/epfl/toolbox/`

2.2 Install Python2.7

If you have a Python2.7 already and you are familiar with commands such as `pip` and `conda`, you can skip this step, otherwise, please read through the rest of this step and see what you need to do.
We highly suggest you install Anoconda to your desktop to get the Python2.7 interpreter, also it helps you manage the packages you need. The download page is here: https://www.anaconda.com/download/#linux You can use `wget` command together with the link address in the download page to get the installation package and `bash` command to install it. Here, we only provide basic and brief instructions for that.

```
wget https://repo.anaconda.com/archive/Anaconda2-5.1.0-Linux-x86_64.sh
bash https://repo.anaconda.com/archive/Anaconda2-5.1.0-Linux-x86_64.sh
```

And then follow the instructions on the screen.

2.3 Install Needed Compilers for SOAP

In this step you will install libraries callable by the `yum` package management system. Follow the commands below.

```
sudo yum install yum-utils
sudo yum install make automake gcc gcc-c++ kernel-devel
sudo yum install fftw-devel fftw-doc
```

Now you are supposed to be able to get all the binaries you need in SOAP package.

2.4 Compile Each Packages

In this section, you will compile each part of SOAP step by step.

- Let's start with `toolbox`. Make sure you can see the `epfl` folder in your current directory.

```
cd epfl/toolbox/src
make clean all
```

(Note: `make clean all` means `make clean` and `make all`) Once this process is finished successfully, you can go to the `bin` folder of `toolbox` to see if you have all the binaries you need.

```
autocorr crosscorr fourier gaussmix histogram ndhistogram trajworks
```

- Now we can move on to `sketchmap`. Go to the corresponding folder and run the `make` comamnd:

```
cd epfl/sketchmap
```

```
make
```
Similar with what we did for toolbox, let's also go check if we have all the binaries we need.
```
dimdist dimlandmark dimproj dimred
```

• Then we continue with `glosim`, note this is `glosim` folder under `epfl`, instead of the `gismo` folder in `sketchmap`. Go to the corresponding directory and run commands in order.
```
cd epfl/glosim/libmatch/lap/permanent-0.0.1/
python2 setup.py build
```
Stay in this folder and run these commands:
```
cp build/lib.linux-x86_64-2.7/permanent.so ../
```
Now go back to `glosim` folder:
```
cd epfl/glosim
cp -r ../QUIP/quippy/build/linux_x86_64_gfortran/lib.linux-x86_64-2.7/quippy
.
```

• Now we can run a simple test:
```
python2 ../glosim.py mol-50.xyz
```
Go to the main folder and run another command related with `sketchmap`
```
mv sketchmap/ sketchmap.ol
git clone https://github.com/cosmo-epfl/sketchmap.git
```
And go to this latest version of `sketchmap` and recompile it:
```
cd sketchmap
make
```

2.5 Notes & Suggestions

In this section, some commands will be provided to help you target at possible problems in failed compilation. Since you are going to need C and C++ compiler for SOAP, here are two commands you can use to check what C and C++ compilers you have.
```
gcc -v
g++ -v
```