How to calculate PDOS using pdosxml utility

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PDOS calculation needs following steps :

1. For PDOS calculation first you have to add related block in fdf file like :

```
%block Projected-density-of-states
-30.00 15.00 0.200 500 eV
%endblock Projected-density-of-states
```

After successful siesta run this will generate systemlable.PDOS in the energy range -30.0 to 15.0 eV in the working directory. Now copy the systemlable.pdos file to ~/siesta/Util/pdosxml

2. Now edit m_orbital_chooser.f90 to select the orbitals whose PDOS you want to calculate For example:

```
wantit = ( orbid%l == 0)
```

will select the "s" orbitals.

```
wantit = ( orbid%l == 0 .and. orbid%z == 1)
```

will select the first "s" orbitals on each n.

```
wantit = ( orbid%l == 0 .or. orbid%l == 1)
```

will accumulate the s and p orbitals on all atoms.

```
wantit = ( orbid%index == 15)
```

will get the PDOS on orbital number 15 (whatever it is).

```
wantit = (orbid%species == "O")
```

will calculate the PDOS of all oxygen atoms.

```
wantit = (( orbid%species == "H" ) .and. (orbid%n == 1) .and. (orbid%l ==0) )
```

will generate the pdos of 1s of H species.

3. Third step is to compile this file using make command :

```
$ make
```

in ~/siesta/Util/pdosxml, this will generate a binary/executable file pdosxml in this directory.

5. Finally for pdos plot you can generate data file using cammand :

$ ./pdosxml systemlable.pdos>XXXXX.dat

Format of the output:

Energy PDOS_up PDOS_down

If the system is not spin_polarized, the third column will be all zeros.

and Process datafile with your favorite graphics program like xmgrace

$ xmgrace XXXX.dat

For each orbitals and species you have to recompile m_orbital_chooser.f90 using make command.

For any doubt during the process you can contact in : drmohanlv@gmail.com