How to calculate DOS using eig2dos utility

After successful siesta run one file systemlabel.EIG is obtained in the working directory in the format (after opening using gedit etc.)

-1.6319

600 1 5

1 -46.04762 -43.90812 -43.69160 -43.57984 -43.24740 -43.19786 -41.44732 -41.37667 -41.10211 -40.91767

-21.83650 -20.91262 -20.63773 -19.97004 -19.78007 -19.08940 -18.83242 -18.72508 -18.71505 -17.98383

-17.84286 -17.78155 -16.69305 -16.66061 -16.30147 -16.16058 -15.75145 -15.48565 -15.26027 -14.90917

-14.67799 -14.61200 -14.38872 -14.18964 -13.83344 -13.57594 -13.11509 -12.94250 -12.68518 -12.66021

-12.48714 -11.83395 -11.72055 -11.41856 -11.36036 -10.86908 -10.84810 -10.60296 -10.40750 -10.06546

-9.86763 -9.64491 -9.51983 -9.38975 -8.85015 -8.78281 -8.57724 -8.30520 -7.77843 -7.75664

-7.54964 -7.42612 -7.35724 -6.92039 -6.79587 -6.62460 -6.58375 -6.42782 -6.12110 -5.88601

-5.80352 -5.61975 -5.56876 -5.37515 -5.31469 -4.89203 -4.63700 -4.28513 -4.08542 -3.97169

-3.63760 -3.47466 -3.42036 -3.26757 -2.88574 -2.56324 -2.42083 -2.36104 -1.98088 -1.79996

-1.74282 -1.56944 -1.41007 -1.32615 -1.17662 -1.02450 -0.87509 -0.61279 -0.54362 -0.40846

-0.30995 -0.17253 -0.09279 0.09317 0.26751 0.36232 0.44781 0.62291 0.75409 0.78615

0.99313 1.05367 1.17839 1.25819 1.30842 1.56811 1.66900 1.77571 1.84073 1.90186

2.17264 2.20937 2.30834 2.42787 2.53925 2.68737 2.83554 2.94064 3.05450 3.25361

3.42410 3.45860 3.51511 3.74287 3.80702 3.96287 4.01518 4.19615 4.28059 4.45806

4.61603 4.72309 4.78004 4.87086 5.03290 5.05939 5.15785 5.28384 5.39228 5.53060

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The highlighted numbers are very important, so here is the explanation of their meaning: -1.6319 eV is a Fermi energy of the system, which has 600 bands, 1 spin component (so it is unpolarized) and 5 k-points each of them is also highlighted.

Before using post-processing tool eig2dos (eig2dos utility is located in *Util* directory of SIESTA. You can compile it using f95 compiler or another one), after Fermi energy please add the following numbers:

eta - I'd call it *precision*, put it less than 1.

Ne - number of eigenvalues, I advise to put it large.

Emin and Emax - interval of energies for which DOS will be calculated (eV).

Put this values exactly on the first line after the Fermi energy. I did it in this way:

```
-1.6319  0.05 1000 -10 10
```

Save and close the file and run eig2dos utility:

```
eig2dos < SystemLabel.EIG | tee dos.dat
```

You may plot the results using *gnuplot* or *grace* program

```
$ xmgrace dos.dat
```

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