To perform a conductivity calculation within the PAW formalism you need to first use a PAW potential and run a ground state calculation with the *prtnabla* variable set to 1 and *prtwfk=1*. This calculates the necessary matrix elements and creates a file named filename _OPT.

The postprocessor *conducti* read the file filename _OPT and calculate the electrical and thermal conductivity.

conducti ¡ filename.files

where *filename.files* contains the input and output filenames.

filename.in contains the following variables in the PAW case:

2 ! 2 for PAW calculations

filename ! generic name of the ground state data files obtained with prtwfk=1

0.073119 0.0000001 5.00 1000 !gaussian width, omega_min, omega_max, nbr pts

Warning the conducti input file is for the moment different when used in the PAW and NCPP modes. With NCPP, the input file is (see */doc/users/conducti_manuel.tex*)

1 ! 1 for norm-conserving calculations

t78o_DS3_1WF4 ! 1st DDK file

t78o_DS4_1WF5 ! 2nd DDK file

t78o_DS5_1WF6 ! 3rd DDK file

t78o_DS2_WFK ! ground state data file obtained with prtwfk=1

9.50049E-04 ! temperature

1.000 ! k point weigth

0.00735 2.0 ! Gaussian and frequency width; omega-max