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 0.0036749 !temperature 1.000 ! K points weight 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 NC modes. In the NC 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