This is an example of calculation of the electron-ion (electron-phonon) coupling parameter in solid gold using XTANT-3 code[[1]](#footnote-1). This should be done in two steps [1]:

1. Dynamical calculation of the irradiation of gold, which creates the dependences of the parameters on time (running XTANT-3).
2. Extracting the coupling parameter as a function of the electronic temperature from the results file (using XTANT\_coupling\_parameter.exe (or XTANT\_coupling\_parameter.x) from !XTANT\_ANALYSIS\_SUBROUTINES directory).

It can be done with the following steps:

Steps from the point I:

1. The files INPUT.txt and dt\_grid.txt must be placed inside of the directory INPUT\_DATA [read the manual !XTANT\_3\_manual.docx or !XTANT\_3\_manual.pdf for more details on the input files]. This example input-file described the irradiation of gold with a single pulse of a gaussian temporal shape with 15 fs FWHM, 10 eV photon energy, and 5 eV/atom of the absorbed dose (and then performs 5 different simulations with parameters randomly set around these defined values, to be averaged in the step II). The number of atoms in the simulation box with periodic boundary conditions (NVE ensemble) is 256 (defined by 4x4x4 orthogonal unit cells, each containing 4 atoms). The time-step is defined in the file dt\_grid.txt (starting with 1 fs, and changing to 0.1 fs before the beginning of irradiation).
2. The files Au\_Au\_TB\_Hamiltonian\_parameters.txt, Au\_Au\_TB\_Repulsive\_parameters.txt, Unit\_cell\_atom\_relative\_coordinates.txt and Unit\_cell\_equilibrium.txt must be placed in the directory Gold (the name given in the first line in INPUT.txt) inside the directory INPUT\_DATA (by default, these files are already present in this directory as distributed together with the XTANT-3 code). They contain the description of the elementary unit cell, the parameters of the TB Hamiltonian (in the NRL form from [2]).
3. Compile the code by calling Make.exe (under Windows) or make (under Unix); it also compiles the post-processing subroutines in the directory !XTANT\_ANALYSIS\_SUBROUTINES [read the manual !XTANT\_3\_manual.docx or !XTANT\_3\_manual.pdf for more details on how to compile the code, which compilers are needed; the compilation file assumes that all the path to compilers are set in your system].
4. Run the compiled code XTANT.exe or XTANT.x. It will create output directory with all the output files and plots created with gnuplot (if it is installed in your computer and the paths to it are set in the system).

Steps from the point II:

1. Once you have the results, stored in 5 directories (filenames starting with OUTPUT\_Gold\_...), place the executable XTANT\_coupling\_parameter.exe (or XTANT\_coupling\_parameter.x) in the same directory with these folders.
2. Run it in the command line with the arguments:

XTANT\_coupling\_parameter.exe -25 30000

Which will use the data after -25 fs (excluding the earlier time with the relaxation of the atomic ensemble, and only including time with the laser pulse is present, hence with evolving the electronic temperature), and create the files with coupling parameter as the function of the electronic temperature up to the temperatures of 30000. Note that this maximal temperature is defined by the absorbed dose in the input-file – it cannot create electronic temperature higher than those reached in the dynamical simulations; if you need higher temperatures, increase the dose in INPUT.txt.

[1] N. Medvedev, I. Milov, Electron-Phonon Coupling and Nonthermal Effects in Gold Nano-Objects at High Electronic Temperatures, Materials (Basel). 15 (2022) 4883. https://doi.org/10.3390/MA15144883.

[2] M.J. Mehl, D.A. Papaconstantopoulos, NRL transferable Tight-Binding parameters periodic table: http://esd.cos.gmu.edu/tb/tbp.html, (n.d.). http://esd.cos.gmu.edu/tb/tbp.html (accessed November 21, 2019).

1. <https://github.com/N-Medvedev/XTANT-3> [↑](#footnote-ref-1)