Thermo_pw a FORTRAN driver for Quantum ESPRESSO routines: progress report 2018

Andrea Dal Corso

SISSA, CNR-IOM, and MaX
Trieste (Italy)

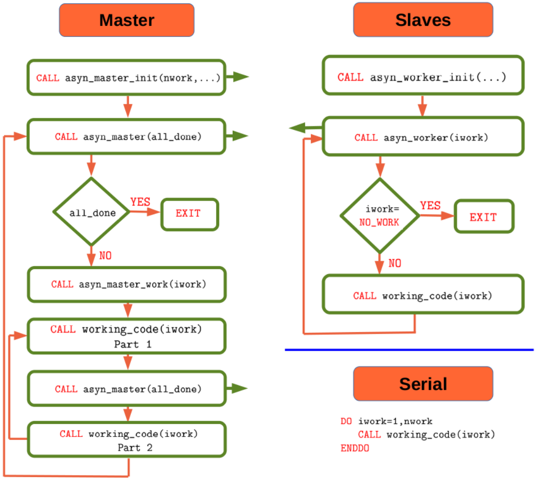
THERMO_PW

Outline

thermo_pw: What is it?

- It is a Fortran driver of the Quantum ESPRESSO (QE) routines that allows the simplification of the calculation of selected material properties.
- It is a Fortran driver that calls `pw.x` and `ph.x` or any QE routine exploiting the image parallelization. The images can communicate in an asynchronous way so the work-load distribution can be done during the run.
- It is a set of pre-processing tools for reducing the number of information that must be provided by the user.
- It is a set of post-processing tools to produce plots directly comparable with experiments.

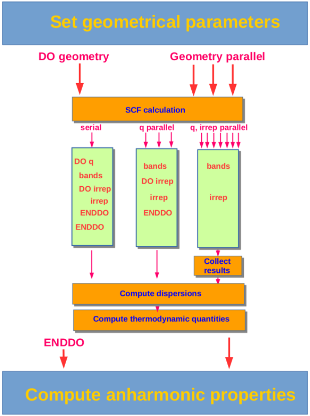
Master/Slave approach to asynchronous control



Serial

```
DO iwork=1,nwork
  CALL working_code(iwork)
ENDDO
```

Phonons and quasi-harmonic thermodynamic

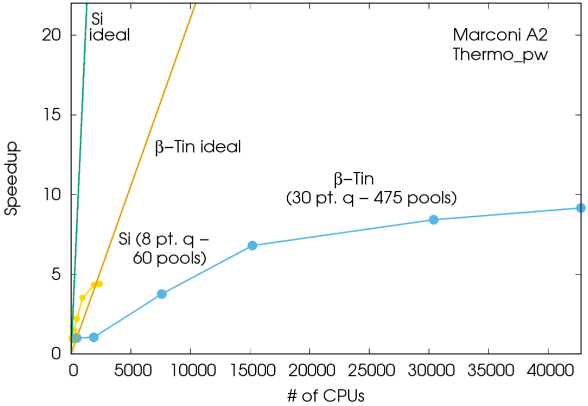


$$F_{ph} = k_B T \sum_{\mathbf{q},\nu} \ln \left[2 \sinh \left(\frac{\beta \hbar \omega_{\mathbf{q},\nu}}{2} \right) \right]$$

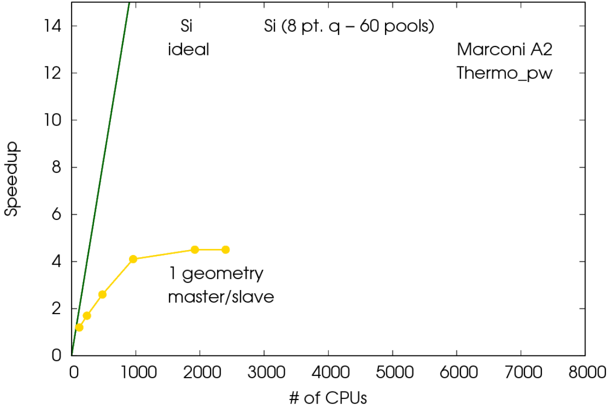
$$F(X,T) = U(X) + F_{ph}(X,T)$$

Minimization of $F(X,T)$ at each T gives $X(T)$.
X are the crystal parameters and
$U(X)$ the total energy at $T=0$.

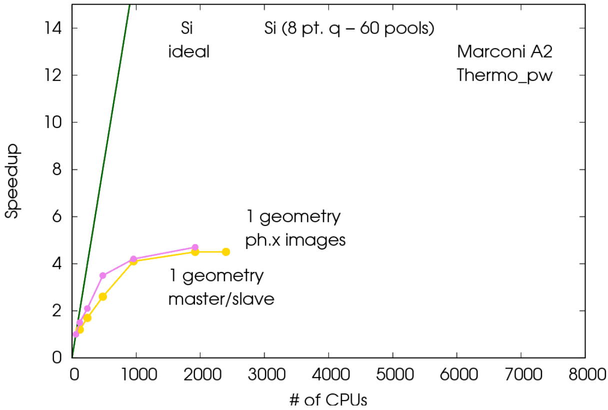
Speed-up of the phonon dispersion calculations with images



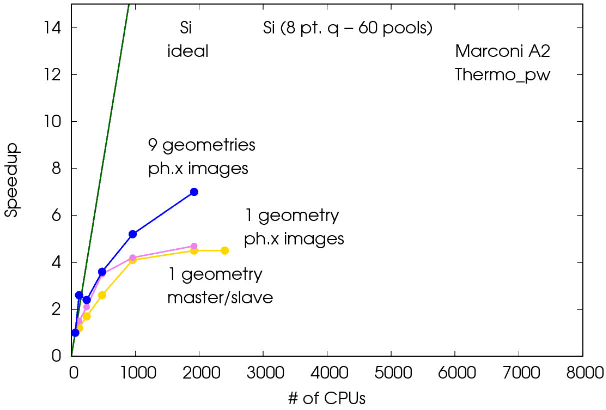
Speed-up of the thermodynamic property calculation with images



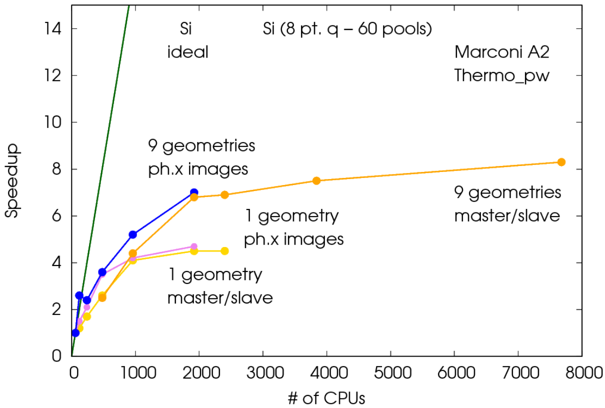
Speed-up of the thermodynamic property calculation with images



Speed-up of the thermodynamic property calculation with images



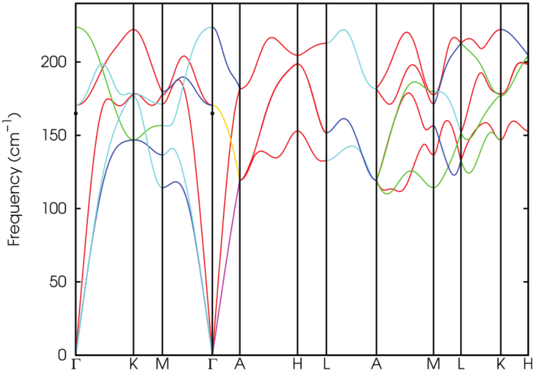
Speed-up of the thermodynamic property calculation with images

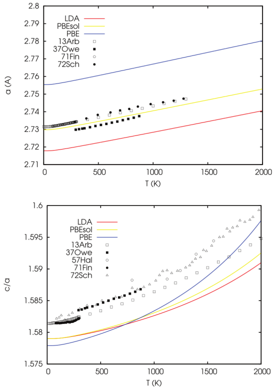


Miscellaneous improvements

- Possibility to recover the phonon calculations even with images.
- max_seconds global variable now can control the asynchronous driver so the master stops all images if the maximum cpu time has elapsed.
- Several bug fix in the bands plots.

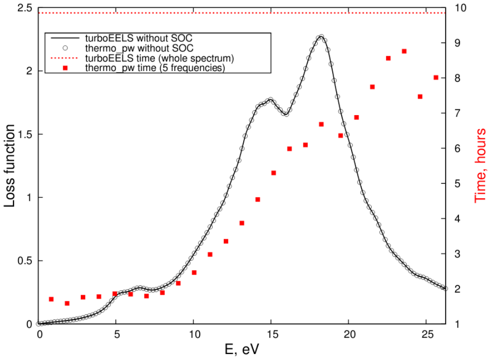
Examples of works made using the quasi-harmonic approximation





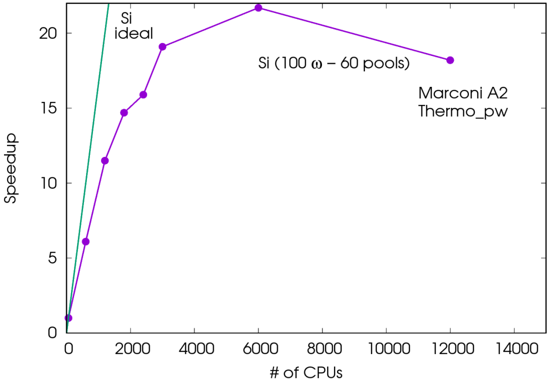
See also:
M. Palumbo and A. Dal Corso, J. of Phys.: Condens. Matter **29**, 395401 (2017).
M. Palumbo and A. Dal Corso, Phys. Status Solidi B: Basic Solid State Physics **254**, 1700101 (2017).

Bismuth loss function: a comparison of turboEELS and thermo_pw



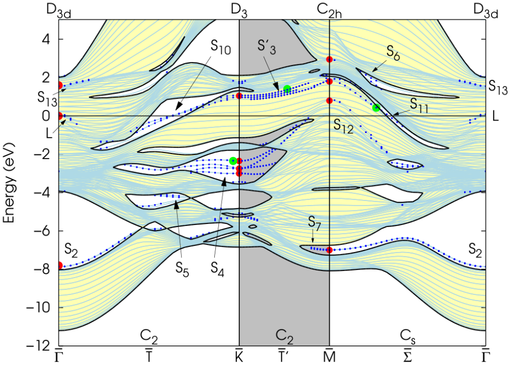
In collaboration with O. Motornyi, M. Raynaud, and N. Vast.

Speed-up for frequency dependent calculations



thermo_pw as a post-processing tool

Fully relativistic surface band structure of Os(0001):



A. Urru and A. Dal Corso, surface science to appear.

Conclusions

- The master/slave approach allows the increase of the speed-up of the phonon dispersions and thermodynamic calculations when the standard parallelization strategies cannot scale further due to the small size of the system.
- The master/slave approach has also several other applications. I have explored the possibility to parallelize the Sternheimer equation over the frequencies, with very good results. This approach, while not competitive with the Lanczos scheme, can be useful in cases in which the latter cannot be applied.
- Several other applications can be envisaged for the next years.