I Parallelization of DFPT calculations

The PHonon package enables calculations of phonon eigenvectors and eigenmodes. This chapter examines the best ways to run PHonon calculations.

I.1 Optimal parallelization parameters for DFPT calculations

As discussed in sec. ??, the PHonon package offers the same three parallelization levels as the PWscf package, namely plane wave, k point and linear algebra parallelization. Furthermore parallelization across q points (so called image parallelization) can be employed, this will be discussed separately in sec. I.2.

I.1.1 k point parallelization

In a first step, the same k point parallelization benchmark as in sec. ?? is run. This is pictured in fig. I.1.

Interestingly, the result from the PWscf calculation on silicon from sec. ?? is not reproduced here: the smallest pool size of 2 is not the one parallelizing best, but instead it is pool size 8. Furthermore, for more than 50 processors, even the biggest pool size 18 shows better scaling than the pool size 2. This is similar to the results in the PWscf benchmark with k point parallelization on the TaS_2 benchmarking system in sec. ??, as the separation between the different pool sizes isn't as clear as in the same benchmark on the silicon benchmarking system.

some more interpretation possible

The wait time of up to 50 % of the wall time shows that the quality of parallelization is not as good as in PWscf benchmark on TaS_2 in sec. ??, there it

which showed values for the runtime in a similar order of magnitude.

reveals that load balancing for phonon calculations is not as easily done as for the electronic structure calculations, at least with just k point parallelization used.

I.1.2 Linear algebra parallelization

I.2 Image parallelization

Better introduction

When using image parallelization, Quantum ESPRESSO outputs a separate time report for every image, so one step is added to the analysis: The total runtime of a calculation is

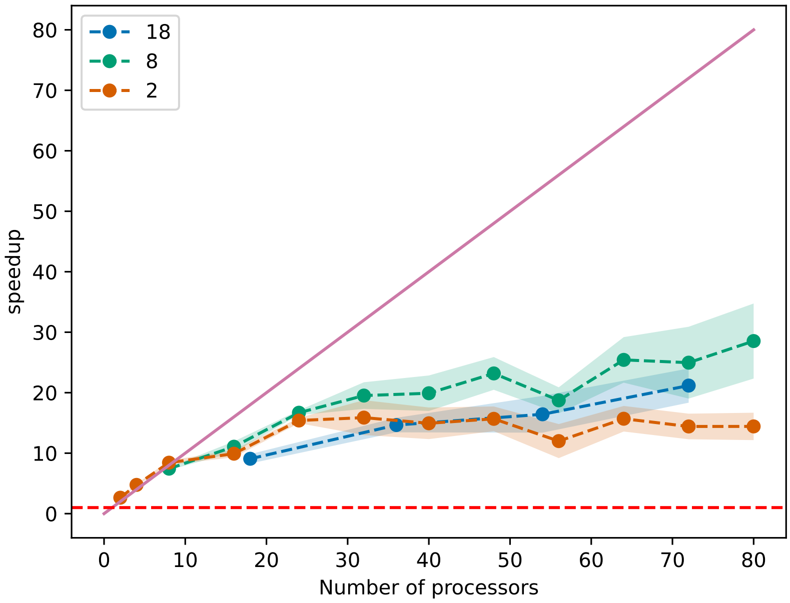

Figure I.1: *Scalability utilizing k-point parallelization for the Si benchmarking system with three sizes of processor pools,* Quantum ESPRESSO compiled with Intel oneAPI 2021.4, `nd 1`

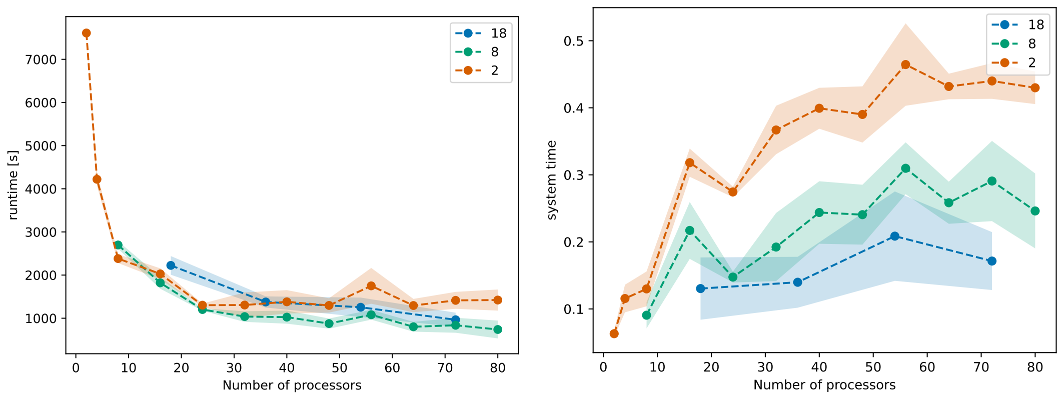

Figure I.2: *Absolute runtime and wait time for the scalability test utilizing k-point parallelization for the Si benchmarking system with three sizes of processor pools,* Quantum ESPRESSO compiled with Intel oneAPI 2021.4, `nd 1`

determined by the longest running image, so speedup will be calculated using that value, but another important measure to evaluate is variation of times between images. This is pictured in fig. I.5.

As the times between images don't vary much, good load balancing between images can be assumed for the silicon benchmarking system.

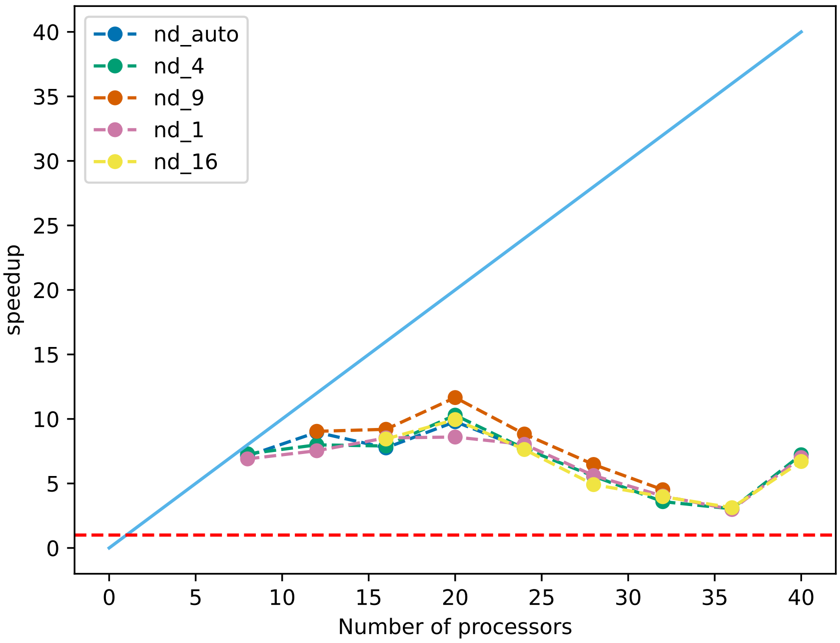

Figure I.3: *Scalability utilizing linear algebra parallelization for the Si benchmarking system,* Quantum ESPRESSO compiled with Intel oneAPI 2021.4, `nk 1`

With the maximum time across images, speedup is then calculated, pictured in fig. I.5.

I.3 Phonon calculations on TaS_2

The results from the last section can be used to estimate good parallelization parameters for a phonon calculation at the Γ point for TaS_2 in the charge density wave phase. The calculations were run on 180 processors, once with the previous established optimal pool size of 36 and once with a pool size of 18 for comparison. The relevant benchmark values for this calculation are listed in tab. I.1.

Table I.1: *CAPTION*

	runtime	wait time
pool size 18	3044 min	0.16
pool size 36	2020 min	0.074

In this calculation the need for a good choice of parallelization parameters becomes especially clear: on the on the same number of processors, with the only difference in the choice of the parameter `nk`, the two calculations have a difference of 17 h.

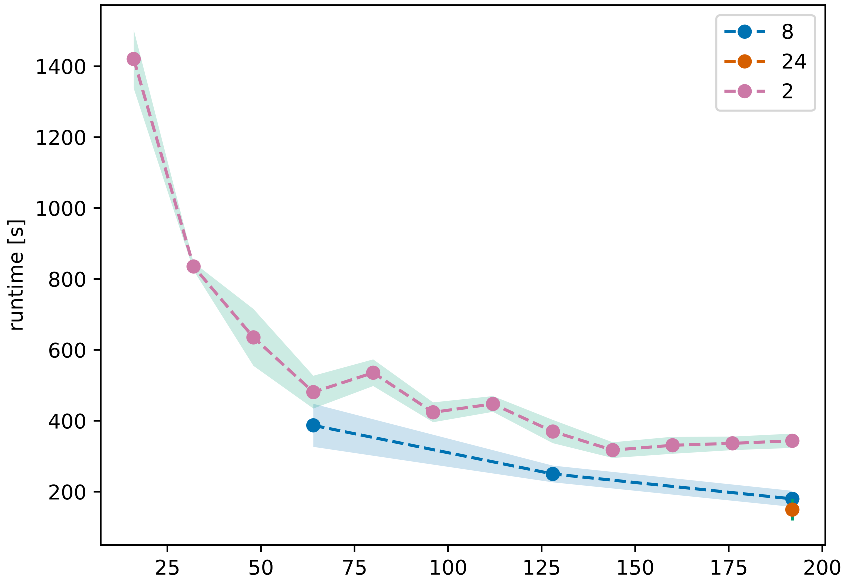

Figure I.4: *Average runtime across images for the scalability test utilizing image and k point parallelization on the Si benchmarking system with three values of* `ni`, QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nk, ni` chosen such that poolsize = 8, `nd 1`

I.4 Conclusion: Parameters for optimal scaling

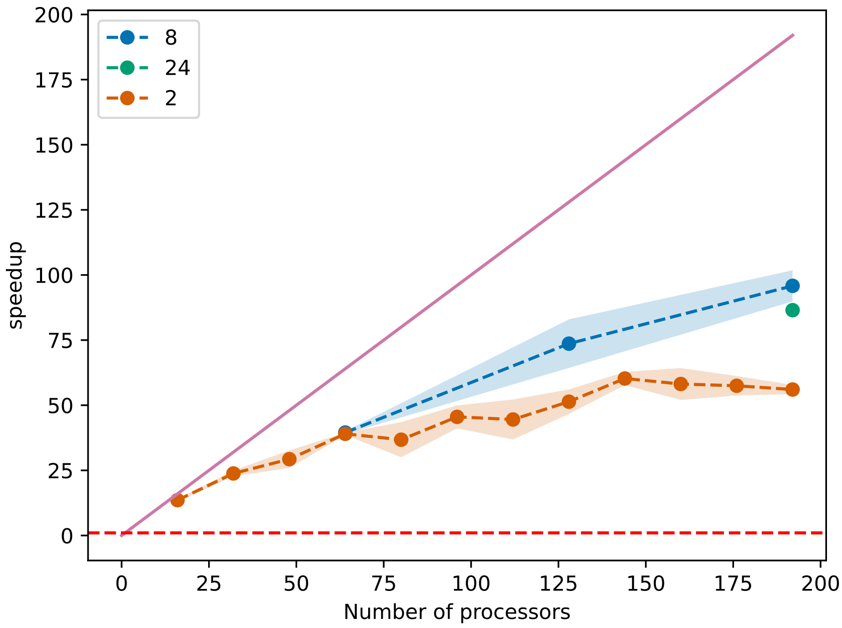

Figure I.5: *Speedup calculated from the longest running image for the scalability test utilizing image and k point parallelization on the Si benchmarking system with three values of* `ni`, QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nk, ni` chosen such that poolsize = 8, `nd 1`

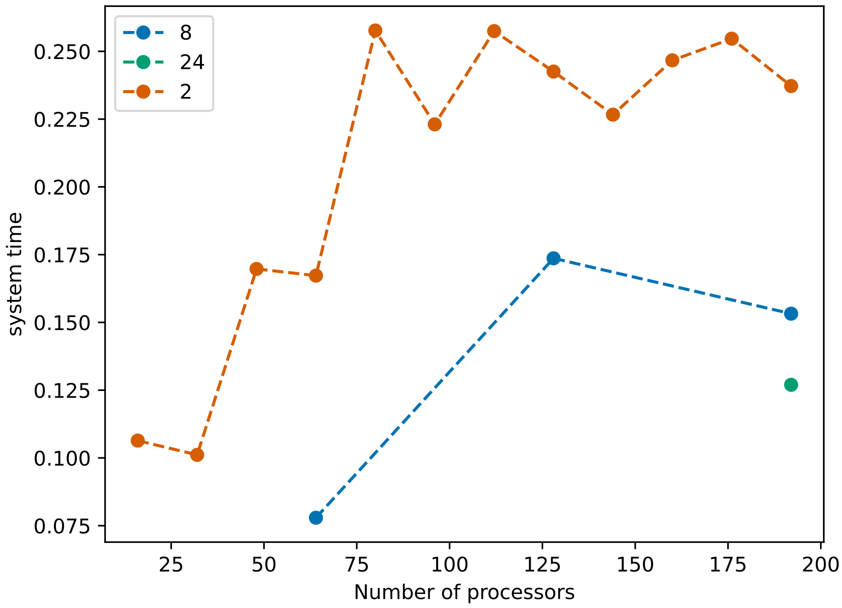

Figure I.6: *Wait time calculated from the longest running image for the scalability test utilizing image and k point parallelization on the Si benchmarking system with three values of* `ni`, QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nk, ni` chosen such that poolsize = 8, `nd 1`