I Parallelization of DFPT calculations

Calculations with the `PHonon` package are significantly more time intensive than `PWscf` calculations, so good parallelization is of the essence to make these calculations manageable.

I.1 Optimal parallelization parameters for DFPT calculations

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 results 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.

The wait time 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 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.4.

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

With the maximum time across images, speedup is then calculated, pictured in fig. I.4.

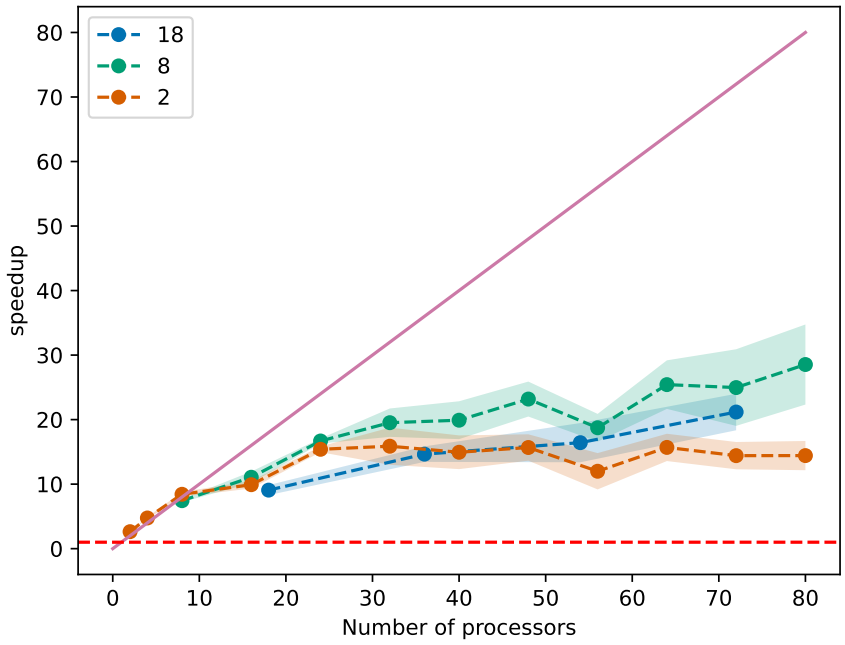

Figure I.1: *Scalability utilizing k-point parallelization for the Si benchmarking system with three sizes of processor pools,* QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nd 1`

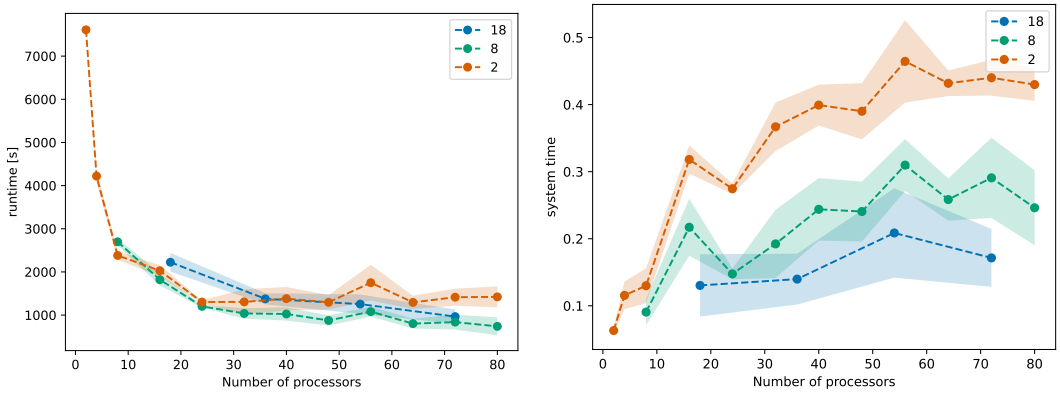

Figure I.2: *Absolute runtime and wait time for the scalability test utilizing k-point parallelization for the Si benchmarking system with three sizes of processor pools,* QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nd 1`

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

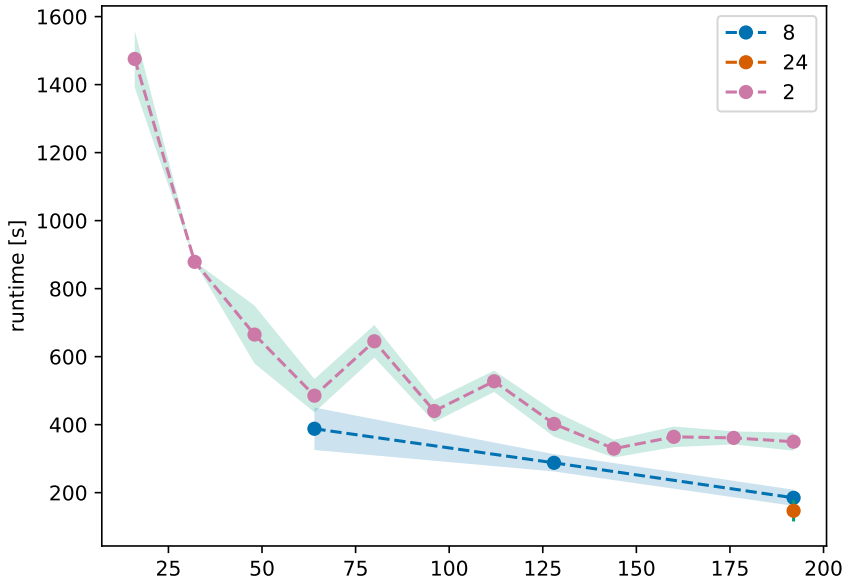

Figure I.3: *Average runtime across images for the scalability test utilizing image and k point parallelization on the Si benchmarking system with three values of* `ni`, QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nk, ni` chosen such that poolsize = 8, `nd 1`

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.

I.4 Conclusion: Parameters for optimal scaling

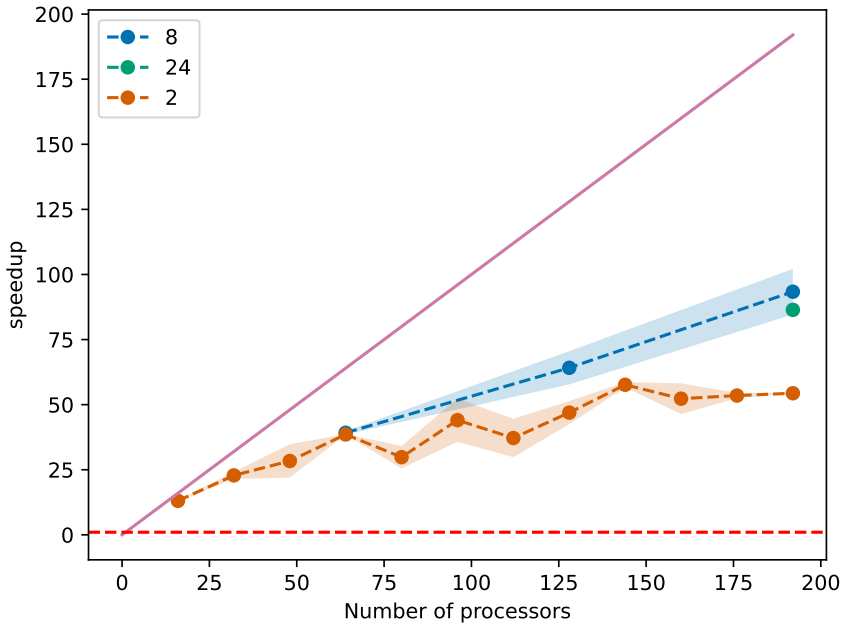

Figure I.4: *Speedup calculated from the longest running image for the scalability test utilizing image and k point parallelization on the Si benchmarking system with three values of* `ni`, QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nk, ni` chosen such that poolsize = 8, `nd 1`

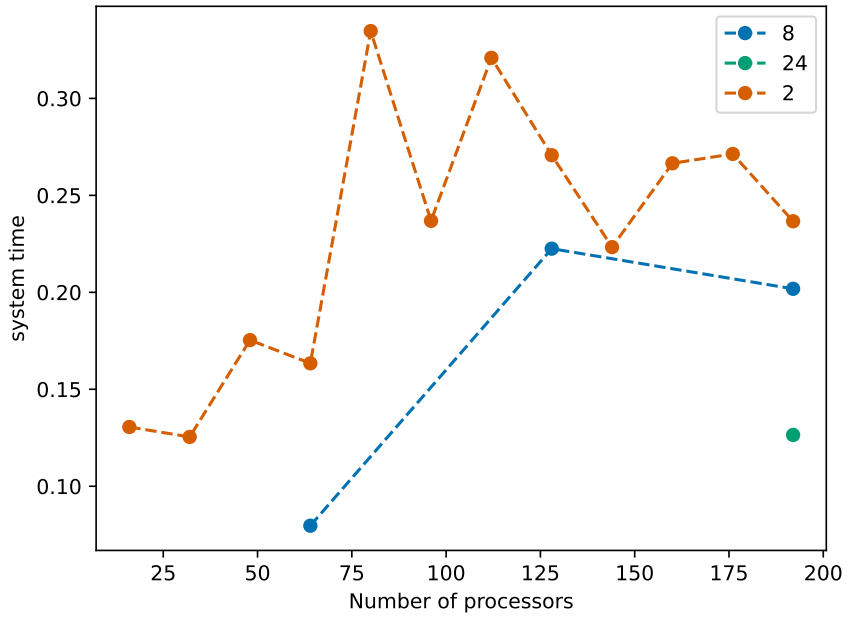

Figure I.5: *Wait time calculated from the longest running image for the scalability test utilizing image and k point parallelization on the Si benchmarking system with three values of* `ni`, Quantum ESPRESSO compiled with Intel oneAPI 2021.4, `nk, ni` chosen such that poolsize = 8, `nd 1`