I Parallelisation of electronic-structure calculations

The `PWscf` (Plane-Wave Self-Consistend Field) package is one of the core modules of QUANTUM ESPRESSO , as many other modules need ground state density and total energy as input. This chapter deals with examining the best ways to run `PWscf` calculations in the `scf` mode.

I.1 First scaling tests

The first step in analysing the scaling of the `PWscf` module is to perform a baseline scaling test without any optimisations appplied. In Fig. I.1 to I.4 two scaling tests on the earlier mentioned benchmarking systems Si and TaS2 are pictured. The tests are run using QUANTUM ESPRESSO 7.0, compiled using the Fortran and C compilers in OpenMPI 4.1.0, without any of the compilation or runtime optimisation parameters mentioned in section **??** used.

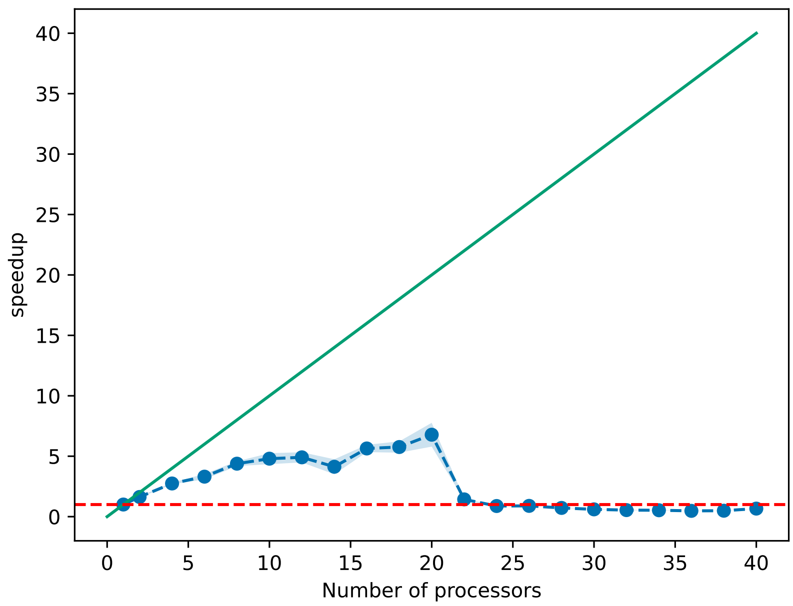


Figure I.1: *Baseline scaling test on the Si benchmarking system* QUANTUM ESPRESSO 7.0, OpenMPI 4.1.0, `nk 1` and `nd 1`

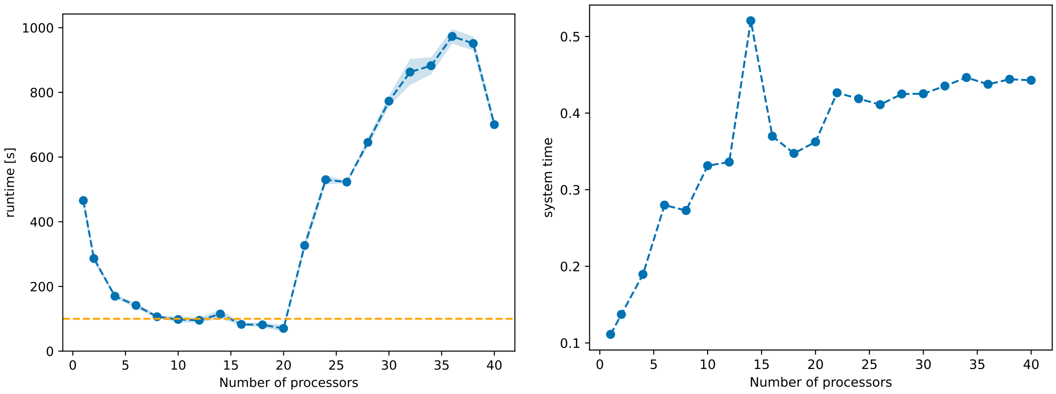


Figure I.2: *Baseline scaling test on the Si benchmarking system* Quantum ESPRESSO 7.0, OpenMPI 4.1.0, `nk 1` and `nd 1`

As discussed in sec. **??**, three different metrics of scalability can be deduced from the time data given by Quantum ESPRESSO :

- runtime: absolute runtime (walltime) of the compute job
- speedup: runtime divided by runtime of the job on a single core
- wait time: percentage of wall time used by system tasks, e.g. writing to disk, etc.

These are pictured in fig. I.1 and I.2 for the silicon benchmarking system.

On a single node, the speedup does scale linearly with the number of processors until around 10 processors, but with a slope of $\frac{1}{2}$ instead of 1 (which would mean ideal scaling). Beyond that number, the slope decreases even more so that a maximal speedup of around 7 is achieved for 20 processors used. One compute node is equipped with 20 cores, so trying to scale the communication intensive calculations beyond that threshold makes the calculations run even slower than on a single core. Interestingly, the wait time plot in I.2 shows that a significant amount (10 % to 40 %) of runtime is taken up by wait time already for less than 20 processors. As discussed in sec. **??**, this is a sign of poor parallelization, which can explain the poor scaling seen in fig. I.1.

Pictured in fig. I.3 and I.4 are the same scaling test run for the TaS2 benchmarking system. Here, the speedup is not taken as runtime divided by runtime on a single core, as the memory required is more than what can be accessed by a single core. Instead, an estimate of the single core runtime is made by multiplying the runtime of the job running on 4 cores by 4. This assumes perfect scaling for 1-4 processors, but the relative scaling is accurate, no matter the accuracy of this assumption.

The scaling test on the TaS2 system shows much better scaling. For up to 20 processors, the speedup follows the ideal scaling with a stark decline with more processors. This is also reflected in the wait time in fig. I.4, as it goes from a small constant value for under 20 processors to some kind of dependence of the number of processors, which hints to communication or bottlenecks being a limiting factor here.

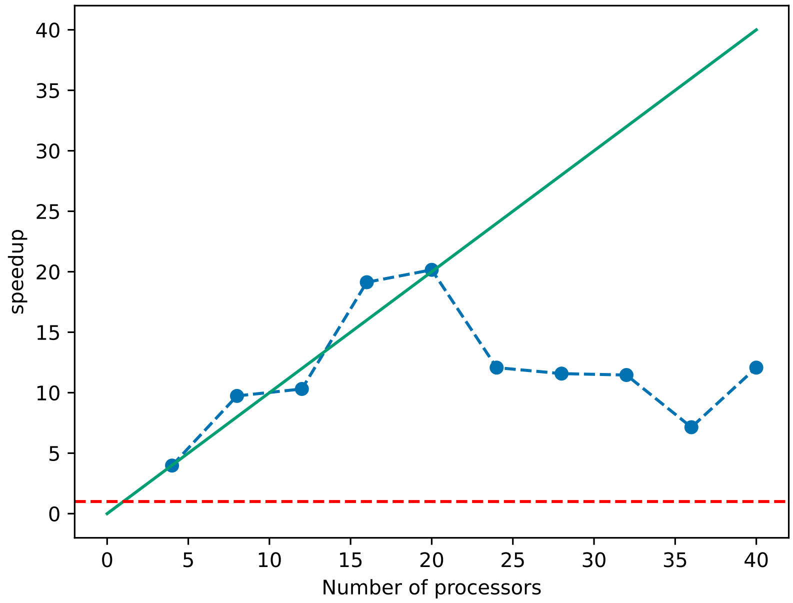


Figure I.3: *Baseline scaling test on the TaS2 benchmarking system* QUANTUM ESPRESSO 7.0, OpenMPI 4.1.0, `nk 1` and `nd 1`

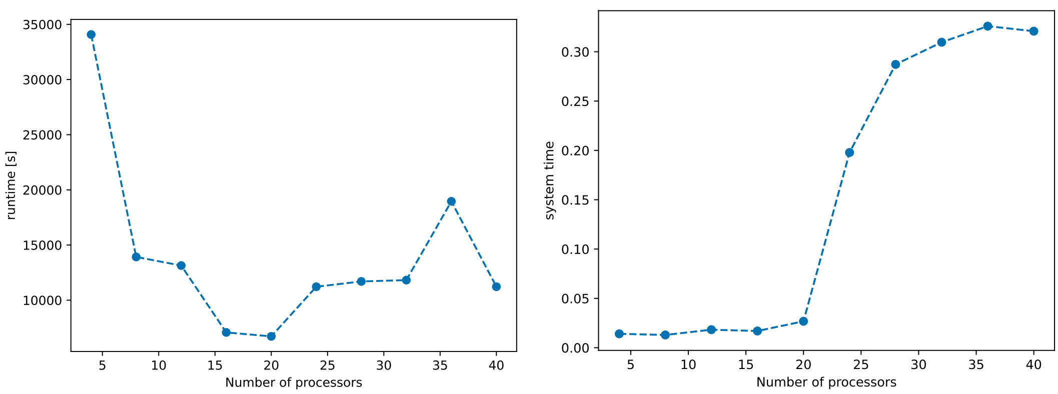


Figure I.4: *Baseline scaling test on the TaS2 benchmarking system* QUANTUM ESPRESSO 7.0, OpenMPI 4.1.0, `nk 1` and `nd 1`

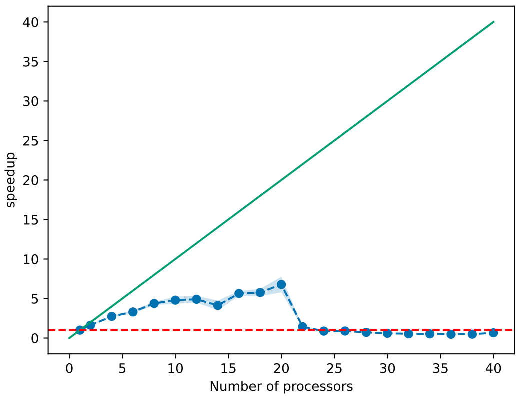
In conclusion, systems with more electrons and by extension bigger matrices and longer iteration times seem to be parallelize better and as such profit more from using more processors than systems with just a few number of electrons.

These scaling tests poses now the question how better scaling over more than one node can be achieved.

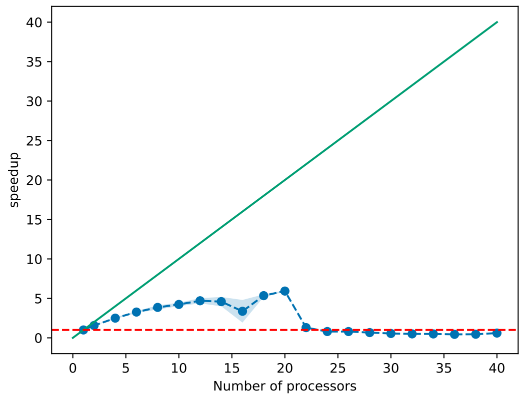
I.2 Testing different compilers and mathematical libraries

A first strategy for solving issues with parallelization is trying different compilers and mathematical libraries. As discussed in sec. **??**, QUANTUM ESPRESSO can make use of a variety of software packages available on the PHYSnet cluster. The benchmarks in **??** are run with the following software combinations:

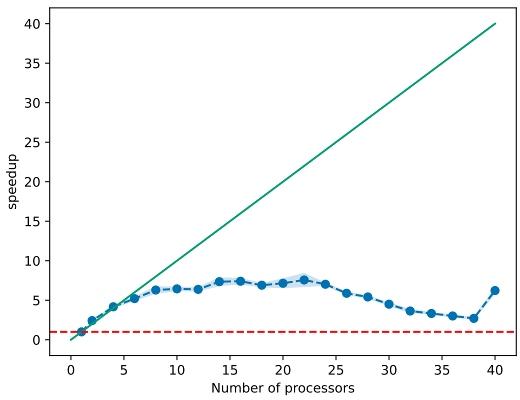
- OpenMPI 4.1.0 and QUANTUM ESPRESSO provided BLAS/LAPACK, so the baseline test discussed in sec. I.1
- OpenMPI 4.1.0, OpenBLAS 0.3.20 and ScaLAPACK 2.2.0
- Intel oneAPI 2021.4



(a) *OpenMPI*



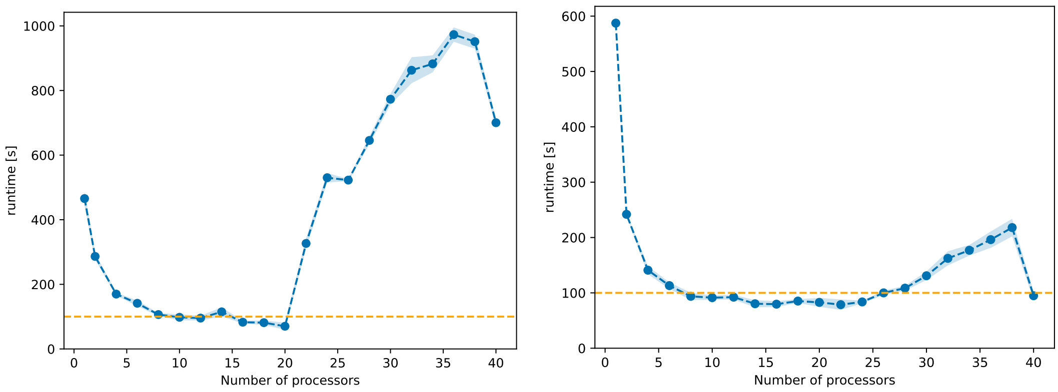
(b) *OpenMPI, OpenBLAS, ScaLAPACK*



(c) *Intel oneAPI*

Figure I.5: *Baseline scaling test Si benchmarking system with different combinations of compilers and mathematical libraries*

Fig. **??** shows that just dropping in another BLAS library (OpenBLAS in this case) does not change the scaling behavior, in contrast to using Intels Intel oneAPI packages. Here, optimal scaling behavior is seen for up to 6 processors. It is however important to also look at the total runtime in this context.



(a) *OpenMPI* **(b)** *Intel oneAPI*

Figure I.6: *Baseline scaling test Si benchmarking system with different combinations of compilers and mathematical libraries*

Fig. **??** shows the absolute runtime for both the OpenMPI and Intel oneAPI benchmarks. This explains the difference in scaling seen in the speedup plots: the runtime on a single core is significantly higher for the Intel oneAPI benchmark, so even though the runtime between both benchmarks is about the same starting from around 10 processors there is a difference in speedup. To assess this more quantitatively, tab. I.1 lists the average runtime for some selected number of processors. Importantly, the runtime for the Intel oneAPI benchmark is faster for smaller numbers of processors (except 1), but only 15 % for 2 cores and even smaller differences for more cores, with the OpenMPI calculation being even a little faster for 20 processors.

Table I.1: *CAPTION*

Number of processors	OpenMPI	Intel oneAPI
1	466 s	587 s
2	286 s	242 s
4	170 s	141 s
10	97.9 s	91.3 s
20	70.2 s	82.8 s

The same benchmark with the Intel oneAPI compiled version of Quantum ESPRESSO is shown in fig. I.7.

For this system, the speedup follows Amdahl's law, discussed in sec. **??** with a linear growth in speedup up to 32 processors with a saturation and only a small gain in speedup with more processors. In contrast to the benchmark with just OpenMPI (fig. I.3) there is no drop in speedup after 20 processors.

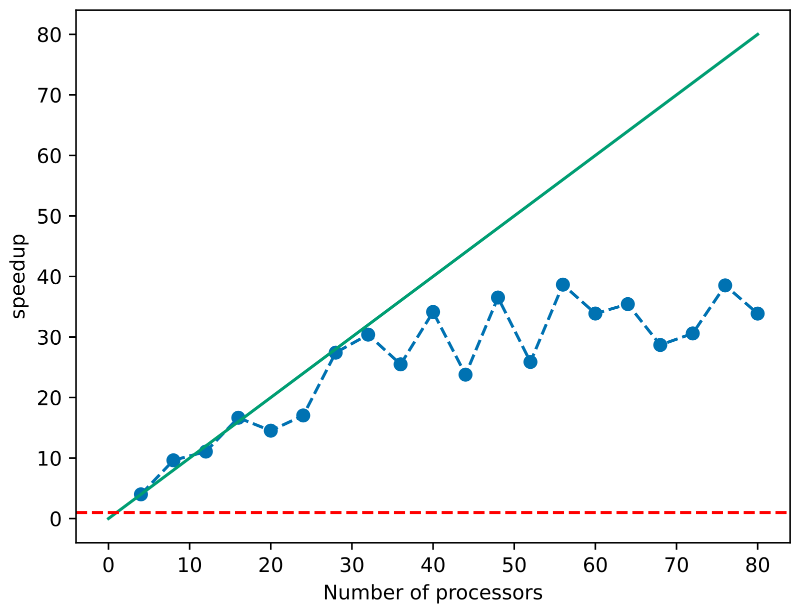


Figure I.7: *CAPTION*

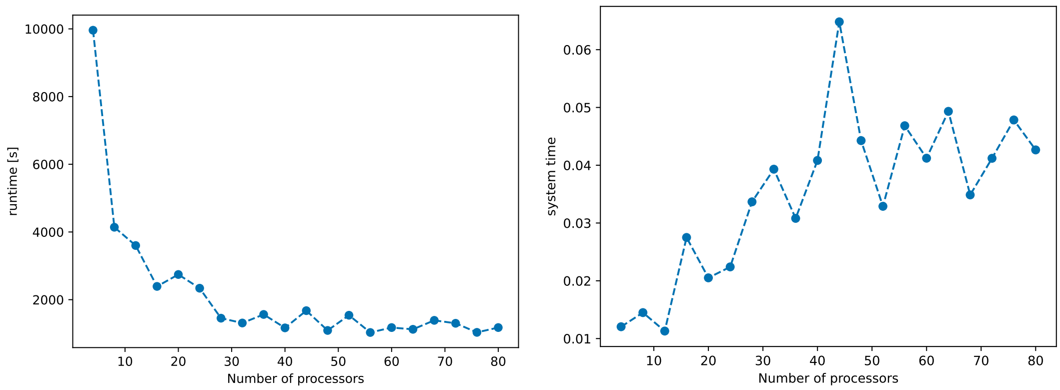


Figure I.8: *CAPTIOn*

TaS2 intel scaling

Moreover, the absolute runtime shown in fig. I.8

This result not only stands for itself as a statement about scaling on a single node, but also provides a basis for scaling beyond the respective optimal ranges of processors for both systems: The k point parallelization explained in sec. **??** can distribute the workload in such a way that processor pools of sizes within this range work on individual k points and as such can provide optimal scaling within one pool while also not losing performance because the pools do not need to communicate with each other in the same order of magnitude as the pools have to communicate within themselves. Keeping the results of this section in mind, at least an for the quality k point parallelization can already be made: For the silicon system, the size of pools should be bigger than 6 processors for optimal scaling and for the TaS2 system they should not be bigger than 32 processors.

I.3 Using the parallelization parameters of Quantum ESPRESSO

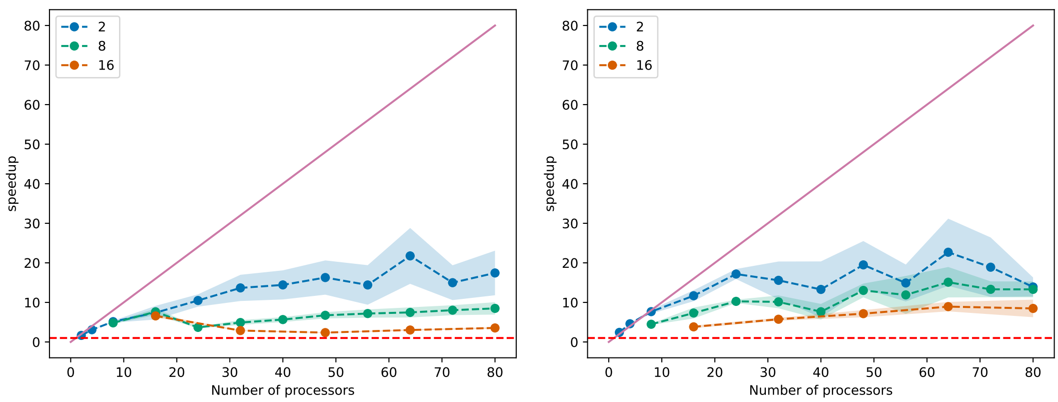
already spoke about k point in the last section, maybe have a better transition here?

As detailed in section ??, QUANTUM ESPRESSO offers ways to manage how the workload is distributed among the processors. In `pw.x` the default plane wave parallelization, k-point-parallelization and linear-algebra parallelization are implemented.

I.3.1 k point parallelization

The benchmark pictured in I.9 is set up as follows: for a given number of processors N_p, the parameter N_k splits the N_p processors into N_k processors pools. As the number of processors in one pool has to be a whole number, only certain combinations of N_p and N_k are possible, for example $N_p = 32$ could be split into processor pools of size 2 with $N_k = 16$, size 8 with $N_k = 4$ or size 16 with $N_k = 2$. This leads to choosing the size of the processor pools as a variable, not the parameter `nk`.

Fig. I.9 shows the scaling for poolsizes 2, 8 and 16 for QUANTUM ESPRESSO being compiled with OpenMPI/Scalapack and Intel oneAPI.



(a) *OpenMPI* **(b)** *Intel oneAPI*

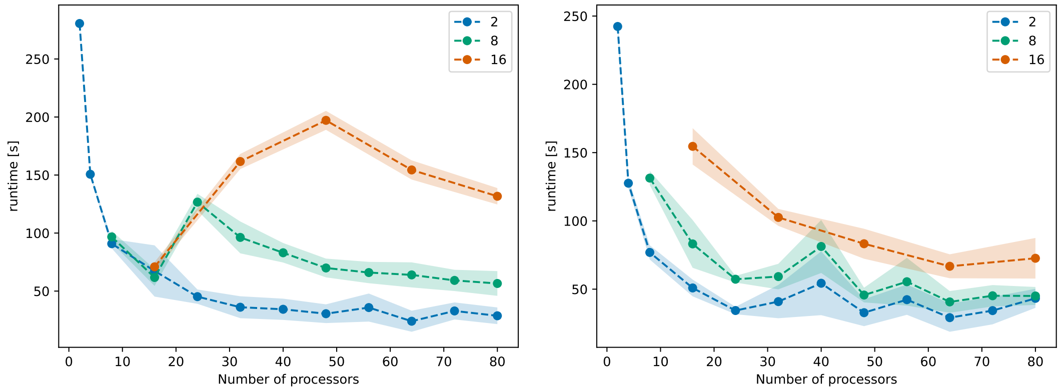
Figure I.9: *Benchmark with k-point parallelization for the Si benchmarking system with 3 different sizes of processor pools*

Fig. I.9 shows that using k parallelization with a pool size of 2 significantly improves the scaling behavior, not only on one node, but especially over more than one node.

more analysis: difference between poolsizes

analyse absolute runtimes

The same scaling test is applied to the TaS2 system in fig. I.11.



(a) *OpenMPI* **(b)** *Intel oneAPI*

Figure I.10: *Benchmark with k-point parallelization for the Si benchmarking system with 3 different sizes of processor pools*

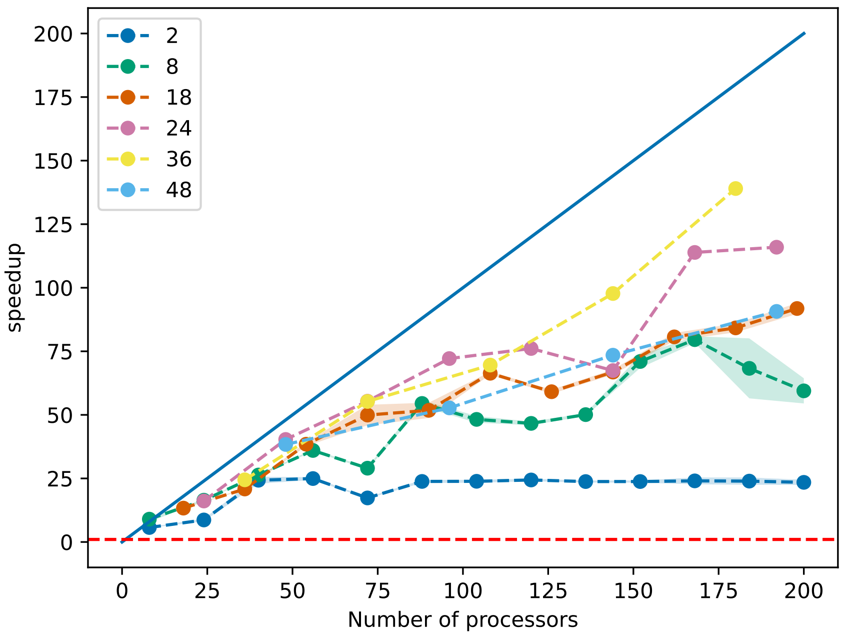


Figure I.11: *Benchmark with k-point parallelization for the TaS2 benchmarking system*

Remarkably, the scaling behavior is swapped in comparison to fig. I.9, as the pool size 2 saturates and the bigger pool sizes show way better scaling behavior. As already alluded to in sec. I.2, the calculations on the TaS2 system profit more from parallelization and as such scale better for bigger pool sizes up until 36 processors in one pool, which is the upper limit established in the benchmark just over the number of processors.

It can also be instructive to look at the idle time for this benchmark to judge the quality of parallelization.

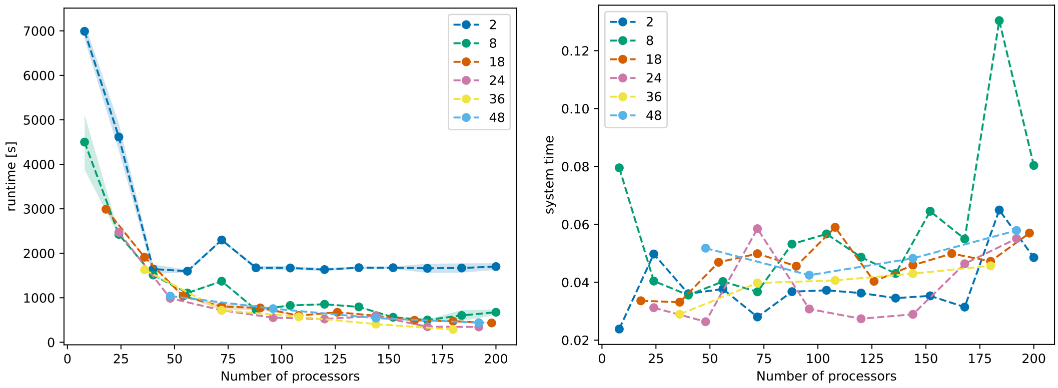


Figure I.12: *CAPTIOn*

Fig. **??** shows a distribution of idle times between about 4 % and 6 % of the whole wall time, without any kind of systemic increase over any range of processors.

more analysis: difference between poolsizes

I.3.2 Linear algebra parallelization

Fig. ?? shows the scaling behavior for different values of the parameter **nd**. Here, nd_auto means that no value for **nd** is specified so QUANTUM ESPRESSO automatically chooses the biggest square number smaller than the number of processors. It is clearly shown that using

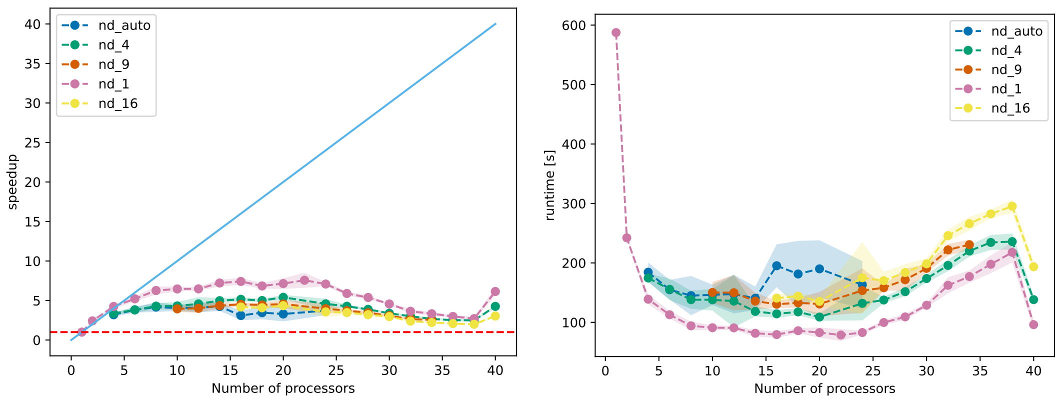


Figure I.13: *Benchmark with linear algebra parallelization for the silicon benchmarking system*

linear algebra parallelization slows the calculation down significantly for the silicon system.

Interestingly, this again is not reproduced for the more expensive TaS2 benchmarking system. Fig. ?? shows a pretty much consistent times across all values for **nd**.

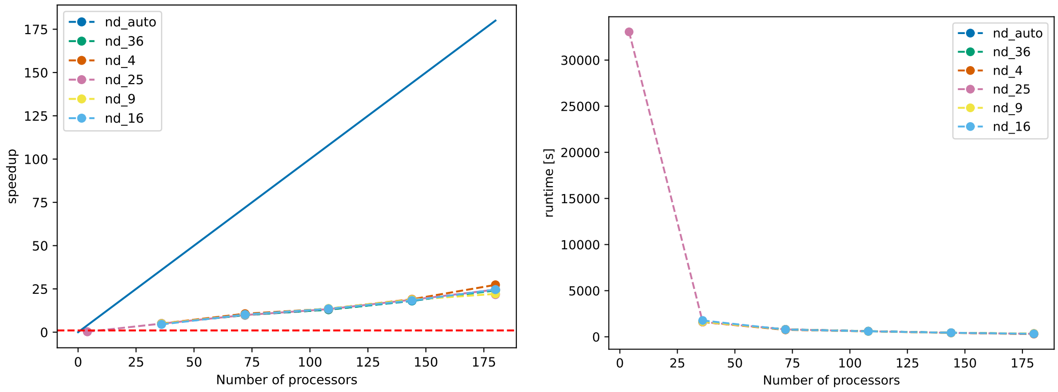


Figure I.14: *Benchmark with linear algebra parallelization for the TaS2 benchmarking system*

Those results are already hinted at in the `PWscf` user guide [1]. Here, in the guide for choosing parallelization parameters, using linear algebra parallelization is recommended when the number of KS states is a few hundred or more. The silicon system has 8 electrons and is as such described with 4 Kohn-Sham (KS) states, the TaS2 system has 153 electrons, so Quantum ESPRESSO uses 92 KS states (in case of metallic materials, the band occupation is smeared around the Fermi energy to avoid level crossings, so more KS states than $\frac{1}{2} *$ (number of electrons) are needed to account for that). Evidently, this number of KS states is on the edge of linear algebra parallelization actually speeding up calculations.

I.4 Comparison with calculations on the HLRN cluster

I.5 Conclusion: Parameters for optimal scaling

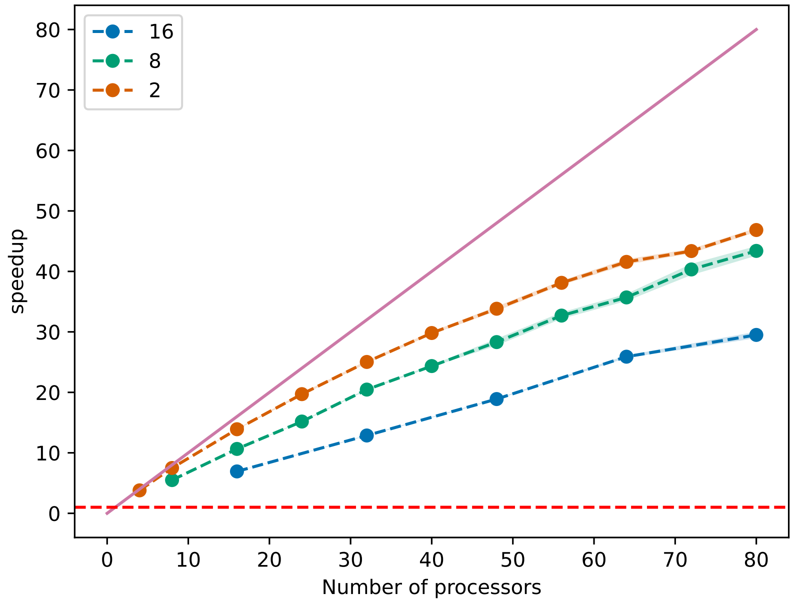


Figure I.15: *CAPTION*

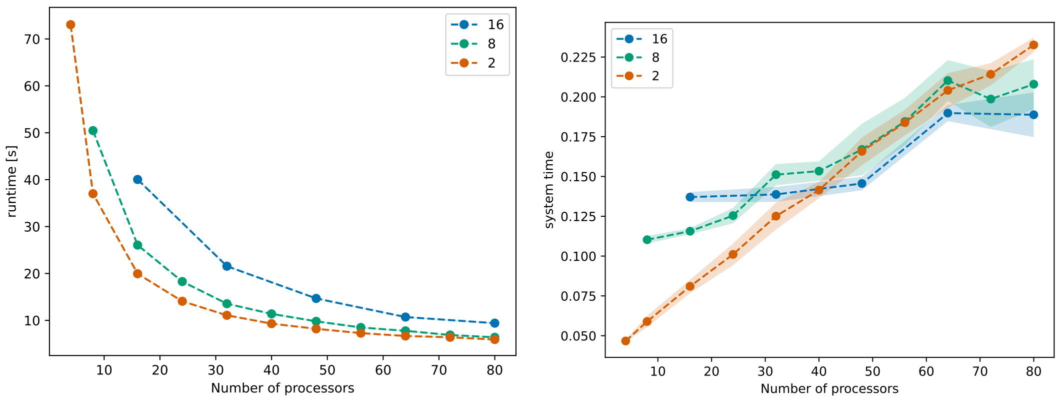


Figure I.16: *CAPTION*

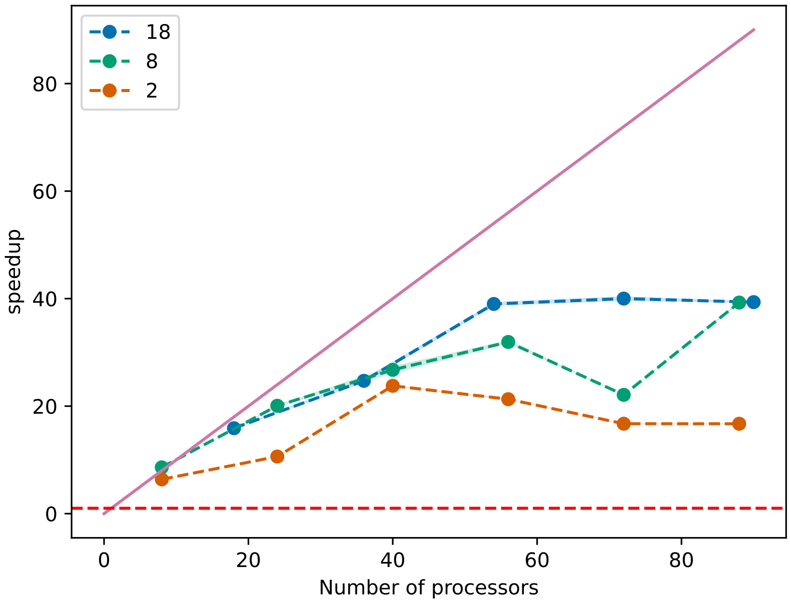


Figure I.17: *CAPTION*

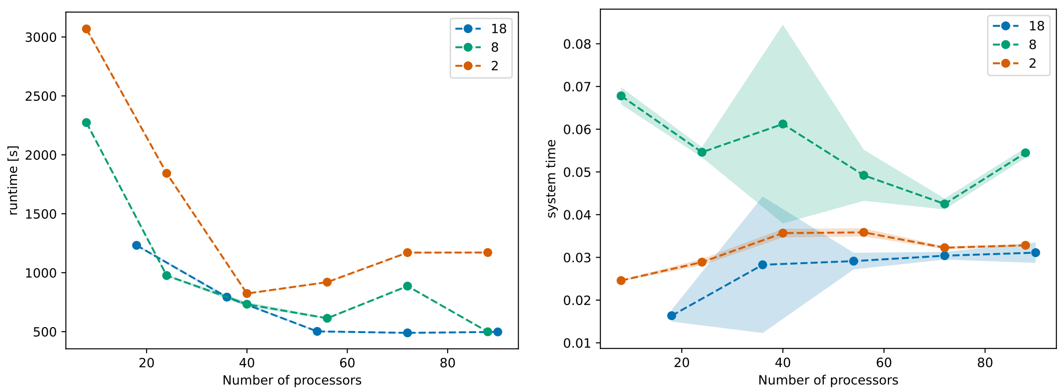


Figure I.18: *CAPTION*