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 TaS_2 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.

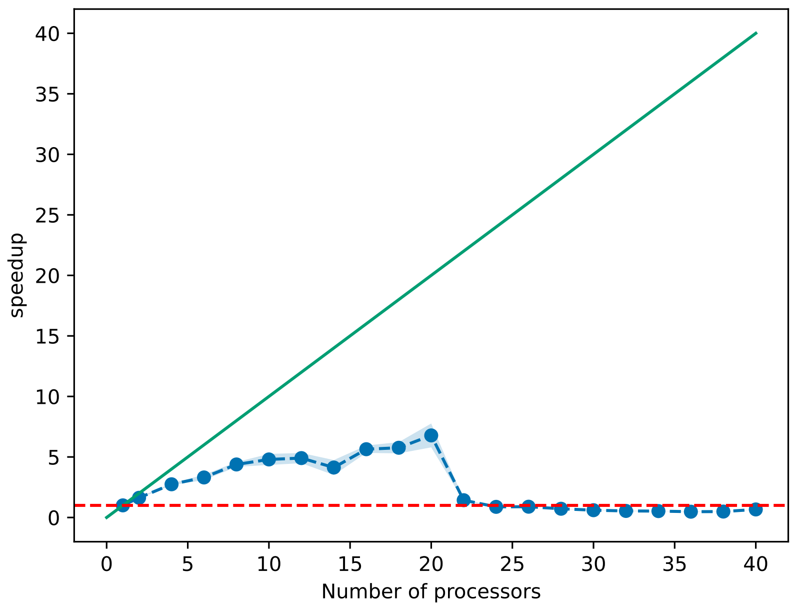


Figure I.1: *Scalability for the Si benchmarking system,* QUANTUM ESPRESSO 7.0, OpenMPI 4.1.0, `nk 1` and `nd 1`

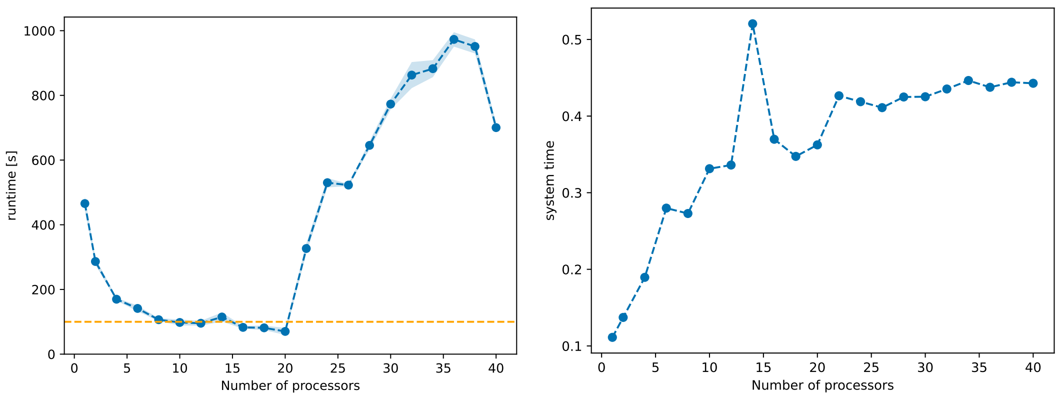


Figure I.2: *Absolute runtime and wait time for the scalability test on the Si benchmarking system,* Quantum ESPRESSO compiled with OpenMPI 4.1.0, `nk 1` and `nd 1`

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 TaS_2 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 TaS_2 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.

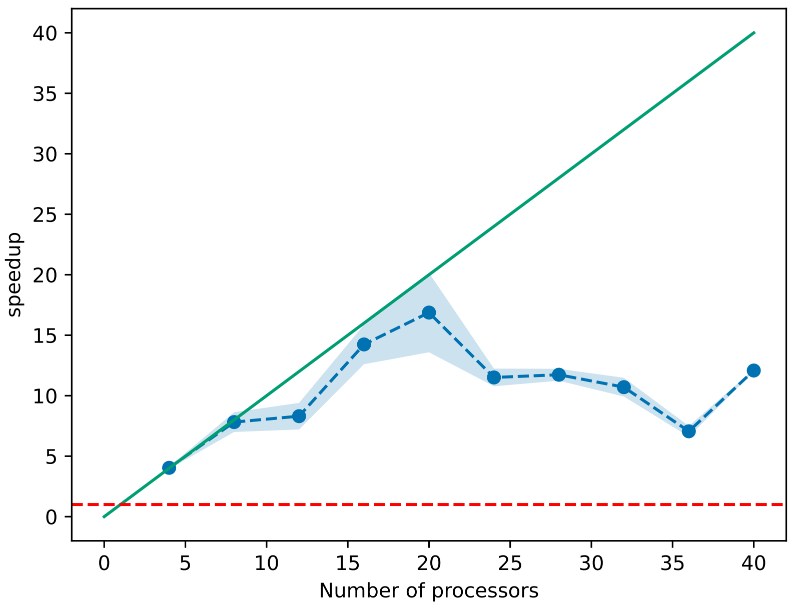


Figure I.3: *Scalability for the TaS_2 benchmarking system,* Quantum ESPRESSO 7.0, OpenMPI 4.1.0, `nk 1` and `nd 1`

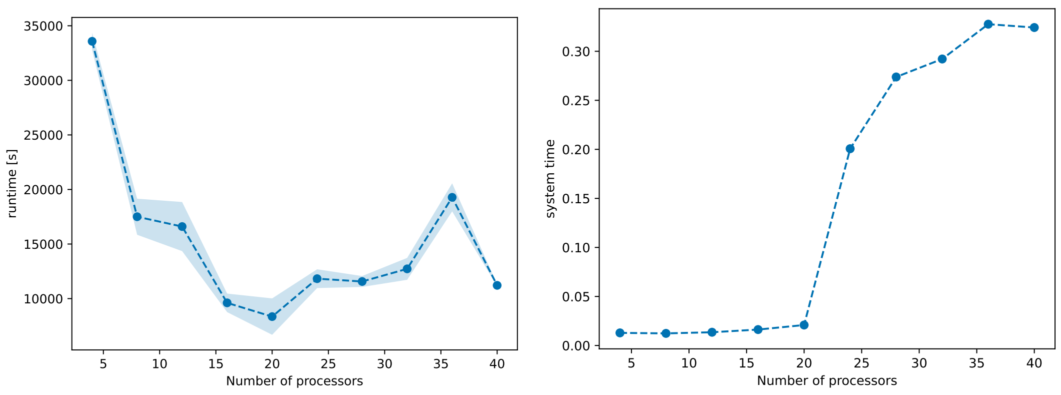


Figure I.4: *Absolute runtime and wait time for the scalability test on the TaS_2 benchmarking system,* Quantum ESPRESSO 7.0, OpenMPI 4.1.0, `nk 1` and `nd 1`

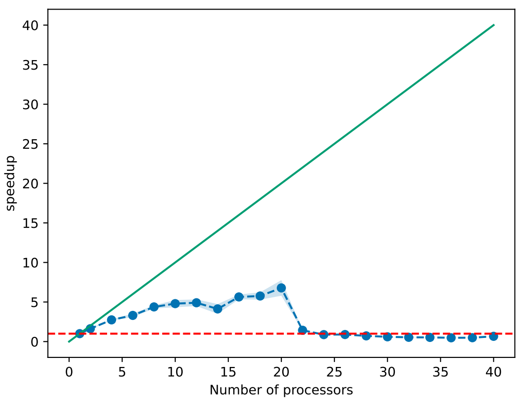
In conclusion, systems with more electrons and by extension bigger matrices and longer iteration times seem to be parallelize better and as such profit more from using more processors than systems with just a few number of electrons.

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

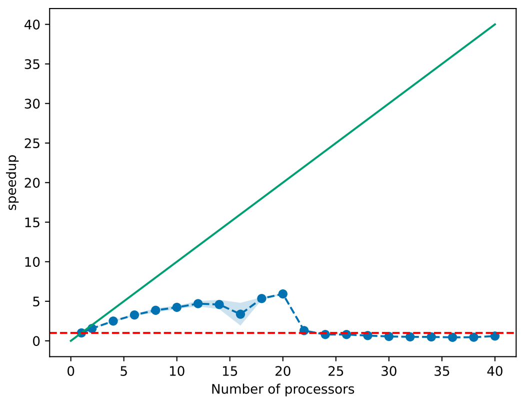
I.2 Testing different compilers and mathematical libraries

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:

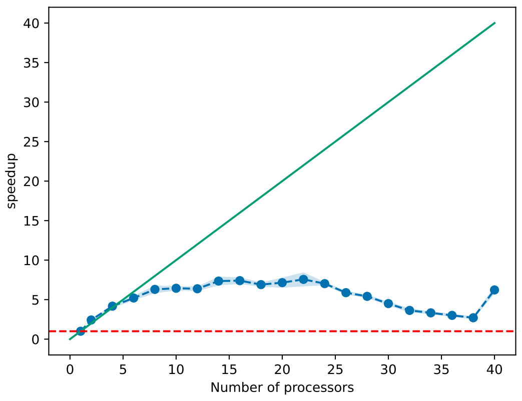
- OpenMPI 4.1.0 and Quantum ESPRESSO provided BLAS/LAPACK, so the baseline test discussed in sec. I.1
- OpenMPI 4.1.0, OpenBLAS 0.3.20 and ScaLAPACK 2.2.0
- Intel oneAPI 2021.4



(a) *OpenMPI 4.1.0*



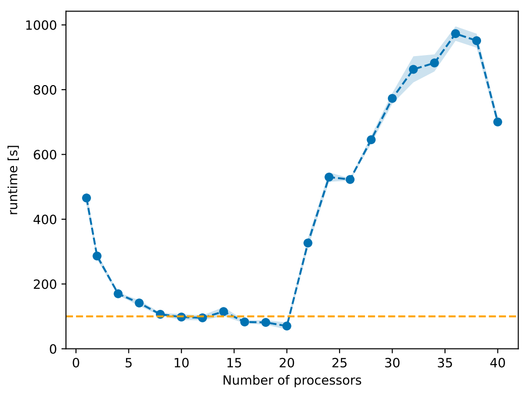
(b) *OpenMPI 4.1.0, OpenBLAS 0.3.20, ScaLAPACK 2.2.0*



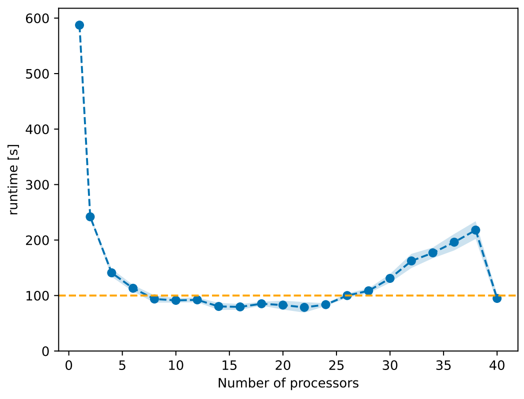
(c) *Intel oneAPI 2021.4*

Figure I.5: *Scalability for the Si benchmarking system with different combinations of compilers and mathematical libraries,* `nk 1` and `nd 1`

Fig. **??** shows that just using another BLAS/LAPACK library (OpenBLAS in this case) with the same MPI version 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 4.1.0*



(b) *Intel oneAPI 2021.4*

Figure I.6: *Comparison of absolute runtimes between Quantum ESPRESSO compiled with OpenMPI and Intel oneAPI for the Si benchmarking system,* `nk 1` and `nd 1`

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: *Selected absolute runtimes of Quantum ESPRESSO compiled with OpenMPI 4.1.0 and Intel oneAPI 2021.4 for the Si benchmarking system,* `nk 1` and `nd 1`

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 and I.8. For this system, the speedup roughly 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. This is remarkable and also a difference to the silicon benchmarking system, where 1 node is a definite upper bound for

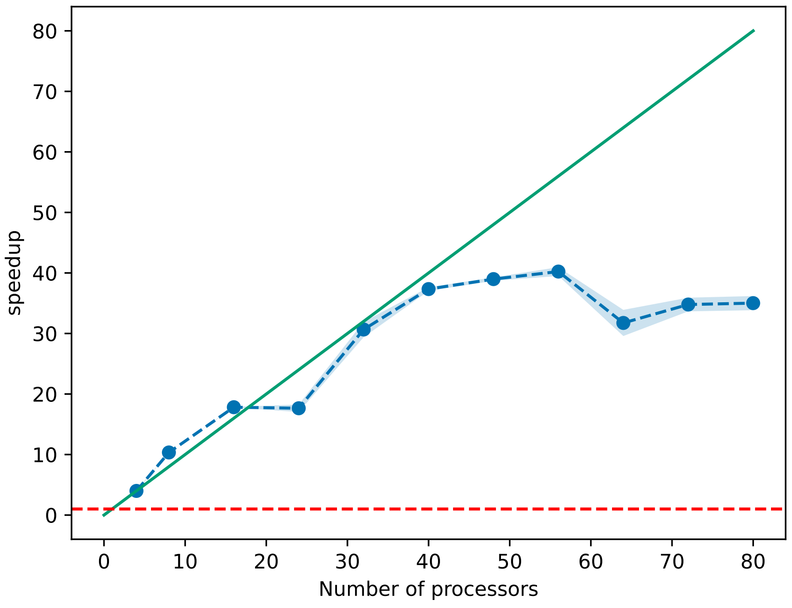


Figure I.7: *Scalability for the TaS_2 benchmarking system,* Quantum ESPRESSO 7.0 compiled with Intel oneAPI 2021.4, `nk 1` and `nd 1`

scalability. An explanation for this behavior can be made with the help of Amdahl's law again. As discussed in sec. **??**, the exact form of the speedup is not dependent on absolute times of parallelized and unparallelized parts of a calculations, but rather the proportion between these two (and can thus be characterized by just the purely serial part s). This means that for a more expensive system such as the TaS_2 benchmarking system, when the absolute time for communication, data distribution and collection stays roughly the same and the time for a single Kohn-Sham (KS) iteration (which can be parallelized) is way longer, the proportion of the purely serial part s gets smaller and the scaling behavior changes significantly.

Moreover, the absolute runtime shown in fig. I.8 shows that the calculations not just scale better than with OpenMPI, but they are significantly faster: whereas the minimum for the OpenMPI benchmark is around 1 h50 min for 20 processors, the Intel oneAPI benchmark averages around 40 min for 24 processors. While the benchmarks on the silicon benchmarking system do not seem to favor one set of compilers over the other, the tests on the TaS_2 benchmarking system clearly show the advantages of using Intel oneAPI on the Intel hardware in the PHYSnet cluster.

The observations on how many processors are optimal for certain kinds of systems not only stand for themselves as a statement about scaling on a single node or a small number of nodes, but also provide 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

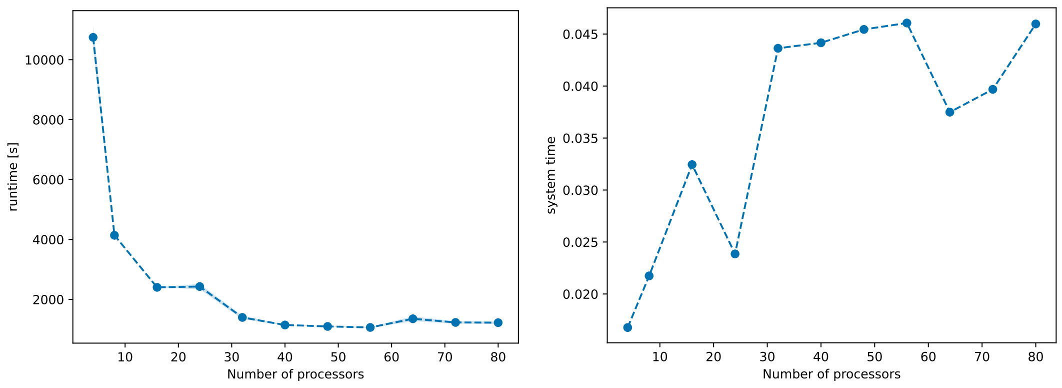


Figure I.8: *Absolute runtime and wait time for the scalability test on the TaS_2 benchmarking system,* QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nk 1` and `nd 1`

to communicate within themselves. Keeping the results of this section in mind, at least an estimate for the quality of k point parallelization can already be made: For the silicon system, the size of pools should not be bigger than 6 processors for optimal scaling and for the TaS_2 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.

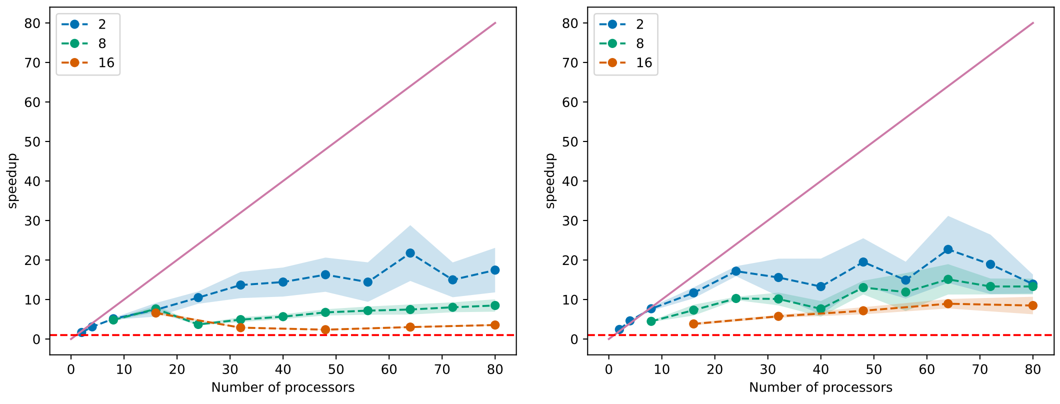
Fig. I.9 shows that using k parallelization with a pool size of 2 significantly improves the scaling behavior, not only on one node, but especially over more than one node.

more analysis: difference between poolsizes

The same scaling test is applied to the TaS_2 system in fig. I.11.

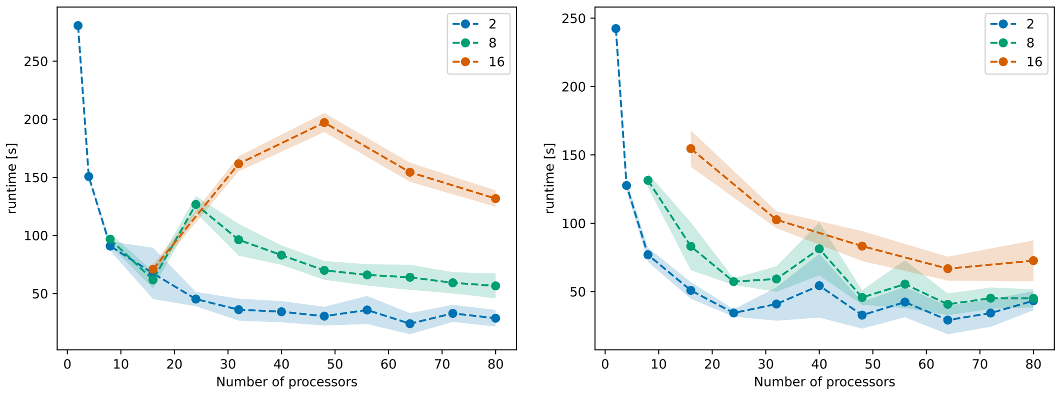
analyse absolute runtimes

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



(a) *OpenMPI 4.1.0* **(b)** *Intel oneAPI 2021.4*

Figure I.9: *Scalability utilizing k-point parallelization for the Si benchmarking system with 3 different sizes of processor pools. The size is determined by the parameter* `nk` *via* size of pools = number of processors / nk



(a) *OpenMPI 4.1.0* **(b)** *Intel oneAPI 2021.4*

Figure I.10: *Absolute runtime for the scalability test with k-point parallelization for the Si benchmarking system with 3 different sizes of processor pools,* `nd 1`

in sec. I.2, the calculations on the TaS_2 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.

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

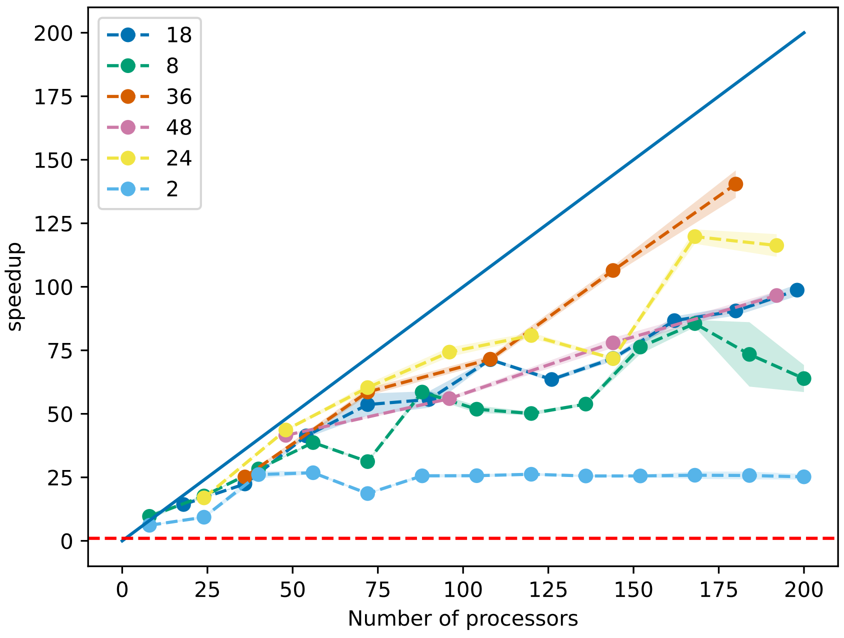


Figure I.11: *Scalability utilizing k-point parallelization for the TaS_2 benchmarking system over a range of processor pools,* QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nd 1`

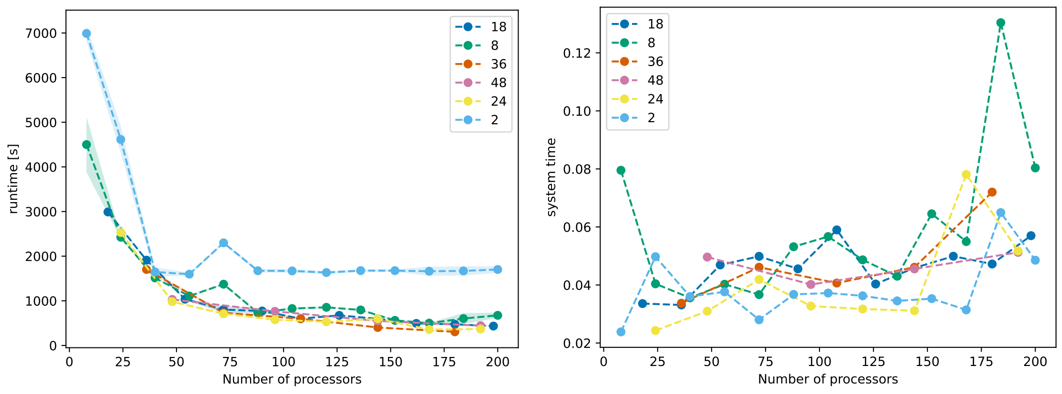


Figure I.12: *Absolute runtime and wait time for the scalability test with k-point parallelization for the TaS_2 benchmarking system over a range of processor pools,* QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nd 1`

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

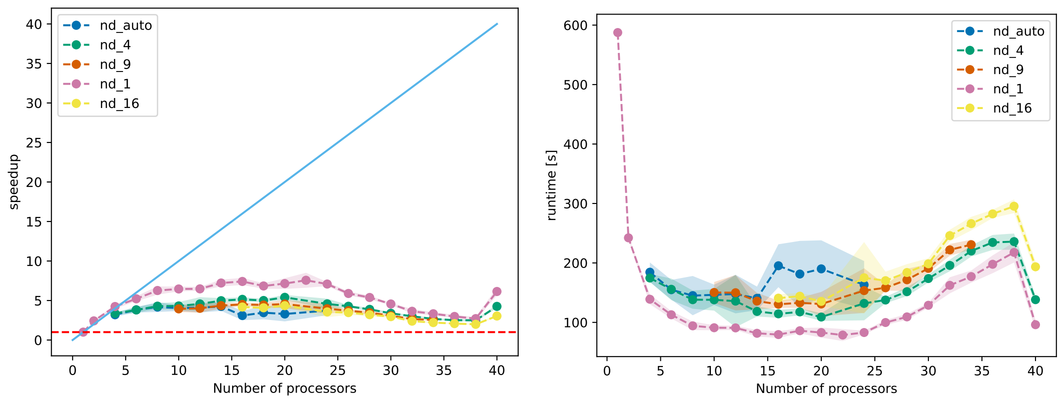


Figure I.13: *Scalability and runtime utilizing linear algebra parallelization for the Si benchmarking system,* QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nk 1`

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

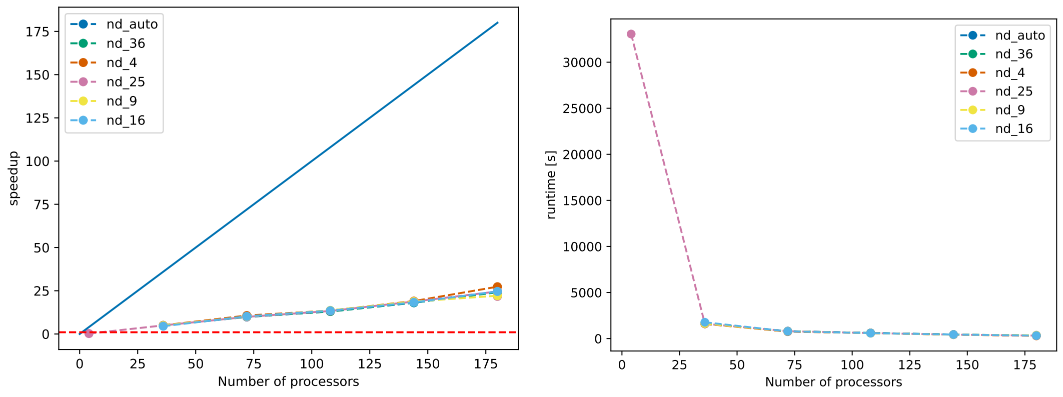


Figure I.14: *Scalability and runtime utilizing linear algebra parallelization for the TaS_2 benchmarking system,* QUANTUM ESPRESSO compiled with Intel oneAPI 2021.4, `nk` chosen such that pool size = 36

Interestingly, this again is not reproduced for the more expensive TaS_2 benchmarking system. Fig. ?? shows a pretty much consistent times across all values for `nd`.

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 KS states, the TaS_2 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

All calculations so far were exclusively run on the PHYSnet cluster and as such are limited by hardware and configuration present in the cluster. To assess this limitation, the k point benchmarks from sec. I.3.1 were run again on the another cluster, the HLRN cluster in particular. The North German Supercomputing Alliance (Norddeutscher Verbund für Hoch- und Höchstleistungsrechnen - HLRN) operates a distributed supercomputer system at the Georg-August-Universität Göttingen and the Zuse Institute Berlin. The current iteration HLRN-IV has nodes with 2 Intel Cascade Lake Platinum 9242 CPUs (48 cores each) and an Omni-Path (Intels proprietary Infiniband competitor) connection between nodes. Quantum ESPRESSO is compiled with Intel Parallel Studio XE Composer Edition 2019 Update 5 (which is the predecessor of Intel oneAPI, bundled without MPI on the cluster) and Intel MPI 2018.5.

Fig. I.15 and I.16 show the benchmarks for the silicon benchmarking system.

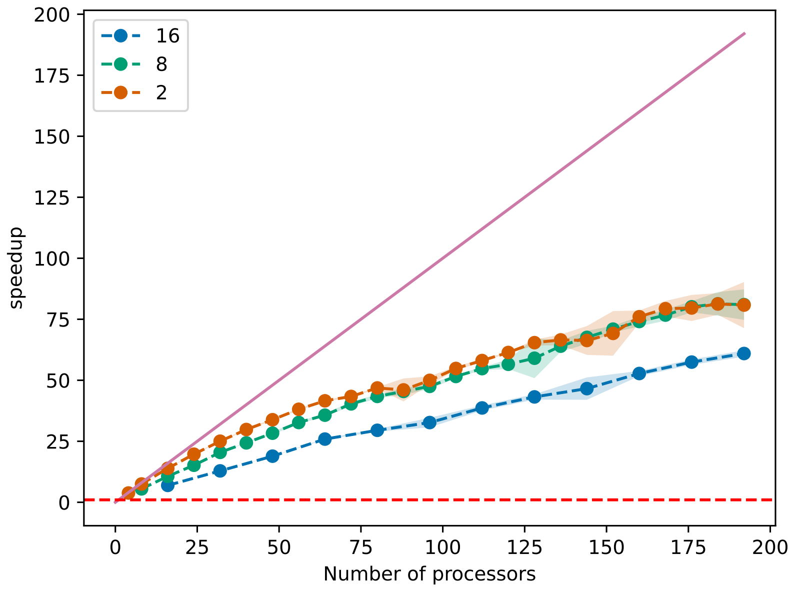


Figure I.15: *Scalability utilizing k-point parallelization for the Si benchmarking system with 3 different sizes of processor pools run on the HLRN cluster,* Quantum ESPRESSO compiled with Intel Parallel Studio 2019u5, Intel MPI 2018.5, `nd 1`

The scaling behavior has some striking differences in comparison with the same benchmarks run on the PHYSnet cluster First of all, speedup and runtimes are very consistent across runs, with only a minimal variance across the whole range of processors. On a single node this is similar to the results from the benchmarks run on the PHYSnet, but on the HLRN cluster this also holds true across two nodes (for more than 96 processors). This is most likely due to the HLRN cluster being equipped with better communication hardware, which is also the reason for the speedup further increasing over two nodes, whereas in the benchmark on the PHYSnet cluster, the maximum speedup of around 20 was already achieved for 24 processors.

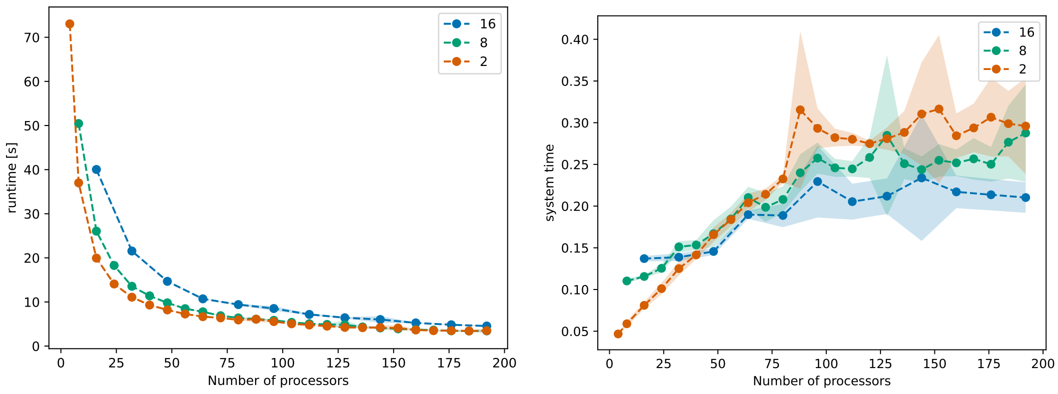


Figure I.16: *Absolute runtime and wait time for the scalability test with k-point parallelization for the Si benchmarking system run on the HLRN cluster,* QUANTUM ESPRESSO compiled with Intel Parallel Studio 2019u5, Intel MPI 2018.5, `nd 1`

wait time HLRN si

A distinction between jobs running across on or two nodes can be made through the wait time though.

Another difference lies in the fact that the pool sizes 2 and 8 show a similar speedup with pool size 16 being a bit worse. This fact shows that while recommendations for parallelization parameters can be qualitatively made based on system size (more expensive system in terms of iterations, absolute runtime, etc. seem to benefit more from bigger k point pools, while smaller pools work best for smaller systems), the optimal size and processor range can vary depending on the compute cluster the calculations are run on.

HLRN analyse für TaS2

Fig. I.17 and I.18 show the benchmarks for the TaS_2 benchmarking system.

I.5 Conclusion: Parameters for optimal scaling

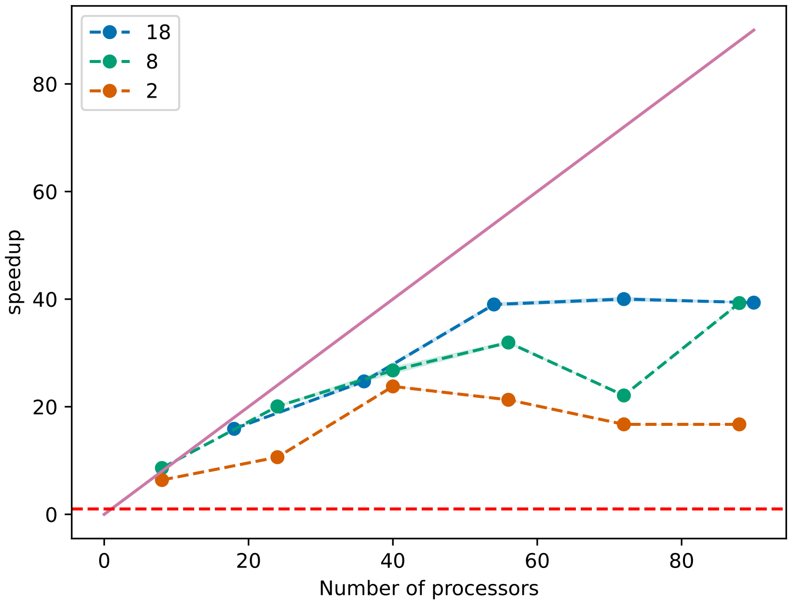


Figure I.17: *Scalability utilizing k-point parallelization for the TaS_2 benchmarking system over a range of processor pool sizes run on the HLRN cluster,* QUANTUM ESPRESSO compiled with Intel Parallel Studio 2019u5, Intel MPI 2018.5, `nd 1`

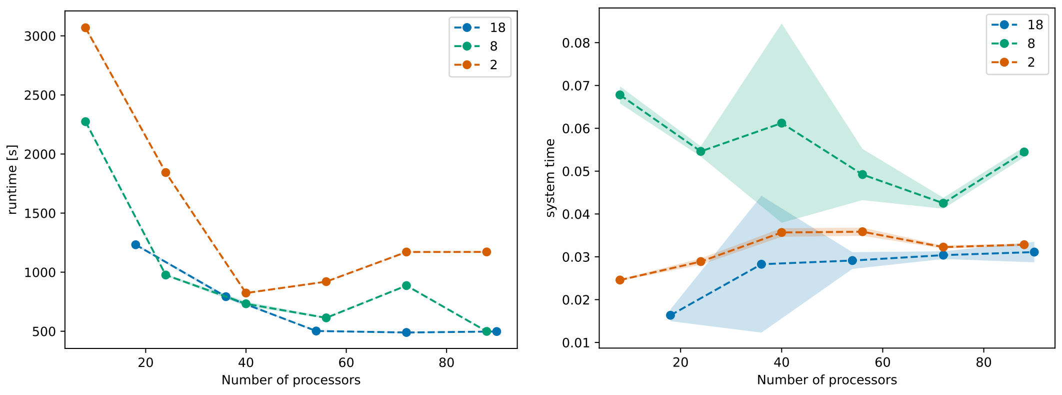


Figure I.18: *Absolute runtime and wait time for the scalability test with k-point parallelization for the TaS_2 benchmarking system run on the HLRN cluster,* QUANTUM ESPRESSO compiled with Intel Parallel Studio 2019u5, Intel MPI 2018.5, `nd 1`