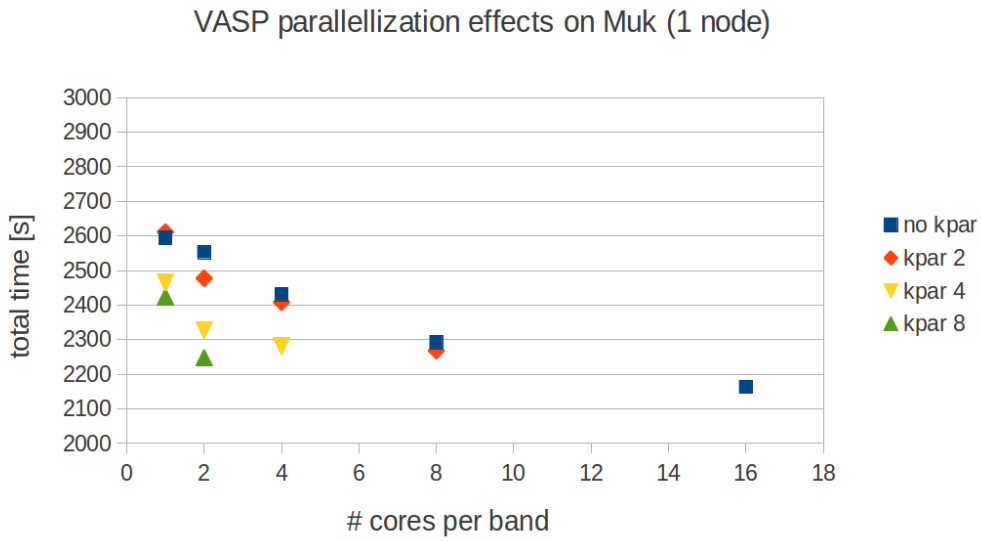
VASP on Muk: performance

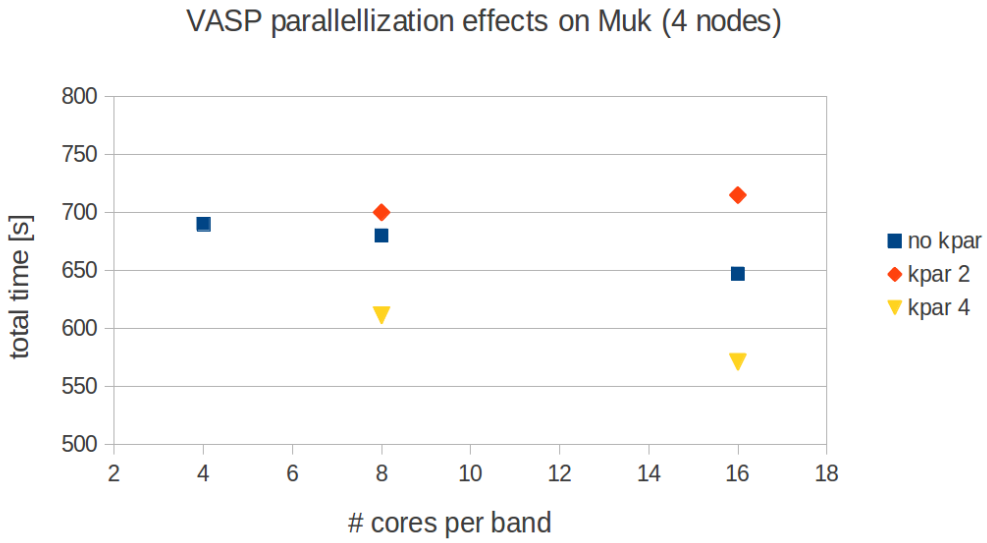
The new VSC Tier1 machine, Muk, consists of:

- 528 computing nodes, with two 8-core Intel E5-2670 (Sandy Bridge) processors each (2.60 GHz clock frequency)
- 64 GB RAM and a 500 GB local 7.2k RPM disk per node
- 400 TB local scratch (DDN SFA10k with 580 of 1 TB 7.2k RPM (data) and 20 of 15k RPM disks (metadata)), accessible through a GPFS-shared file system
- a Mellanox Connect-X FDR Infiniband network
- 4 login nodes, each identical to a computing node

Test problem: Pt induced nanowie on Ge (100) with 320 electronic bands and 8 irreducible k-points in a 3-step geometry optimization (LDA, 345 eV cut-off)

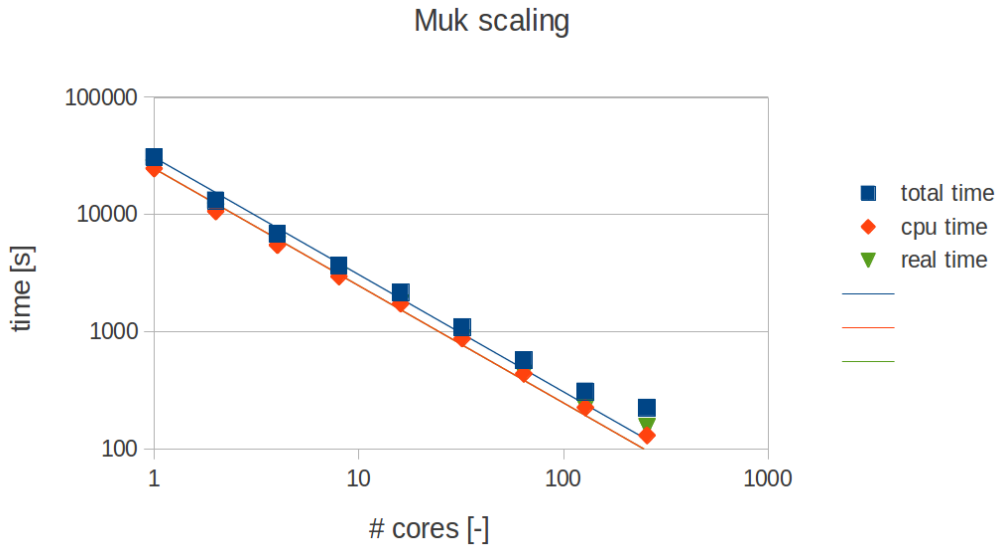
1 Optimal settings for VASP

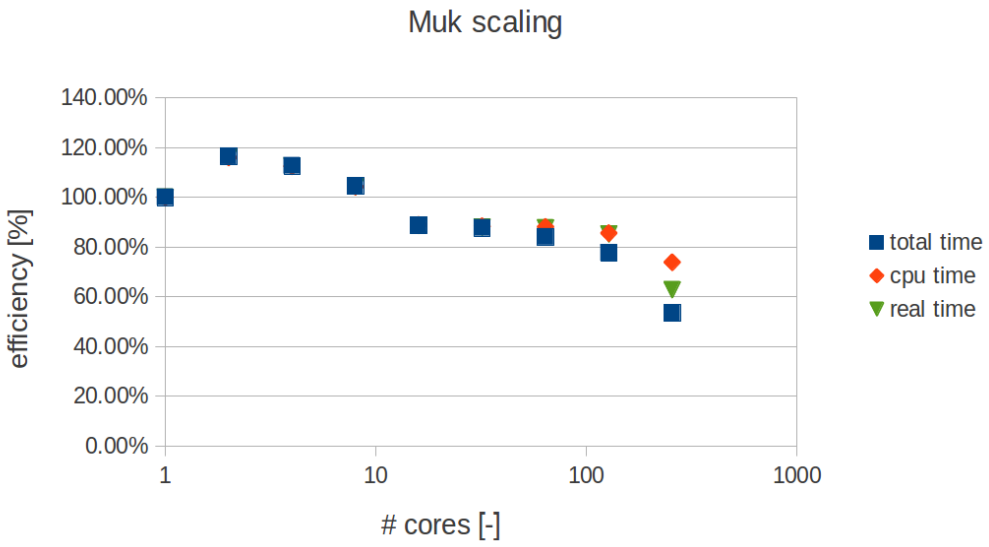




The total duration of a computational run decreases as the number of cores per band (within a node) increases. The optimal setting for NPAR is hence equal to the number of nodes. K-point parallellization is very efficient, but for multinode calculations, it is best to use it only when more than 2 k-points are computed simultaneously. The optimal setting for KPAR is hence equal to the number of k-points, or as large as possible (if this number is larger than 2).

2 Muk scaling





Muk displays an almost ideal scaling behaviour up to 100 cores. For even more cores, the cpu time keeps scaling reasonably well, but other issues, such as data transfer, consume increasingly more time.

3 Limitations

Preliminary tests with VASP have been performed using cells with up to 1728 atoms (CuZr supercells). 1000-atom structures can still be computed on 512 cores (32 full nodes), but for the 1728-atom cells, it is already necessary to revert to hybrid-mode calculations (partial use of the node), in particular 512 cores or 128 partially filled nodes.

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[1] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11 169 (1996).
If the PAW-version is used, reference will be made to
[2] G. Kresse and D. Joubert, Phys. Rev. **59**, 1758 (1999).
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