Experiences of choosing number of cores and NPAR for VASP 5.2 on HECToR

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This document summarises the experience I have had in running VASP 5.2 on HECToR. It may be of some use in helping to select the number of cores you should run on and the value of the VASP parameter NPAR.

Note: I do not provide any guidance beyond that available in the VASP manual on whether to set LPLANE to TRUE or FALSE.

Note: All the benchmarks I have used use the PAW method to describe the core electrons so I have not evaluated the performance of the US pseuopotential method.

Note: All runs were performed using the version of VASP 5.2 that can be accessed by loading the `vasp5/5.2_dev` module on HECToR Phase 2a.

Benchmark Systems

Bench 1: Li defect in ZnO (GGA)

- Γ-point
- 64 atoms
- GGA functional
- Single-point SCF

Bench 2: Li defect in ZnO (Hybrid-DFT)

- Γ-point
- 64 atoms
- GGA functional
- Single-point SCF

Bench 3: TiO_2 5×5×5 Supercell

- Γ-point
- 750 atoms
- GGA functional
- 6 SCF cycles

Results

Bench 1: Li defect in ZnO (GGA)

Γ-point code. For this calculation I would recommend using 128 cores and NPAR = 16.

Cores	NPAR	Time / s
16	1	115
16	2	106
16	4	123
32	2	63
32	4	60
32	8	68
64	2	59
64	4	41
64	8	49
128	8	46
128	16	25
128	32	29
256	16	25
256	32	22
256	64	25

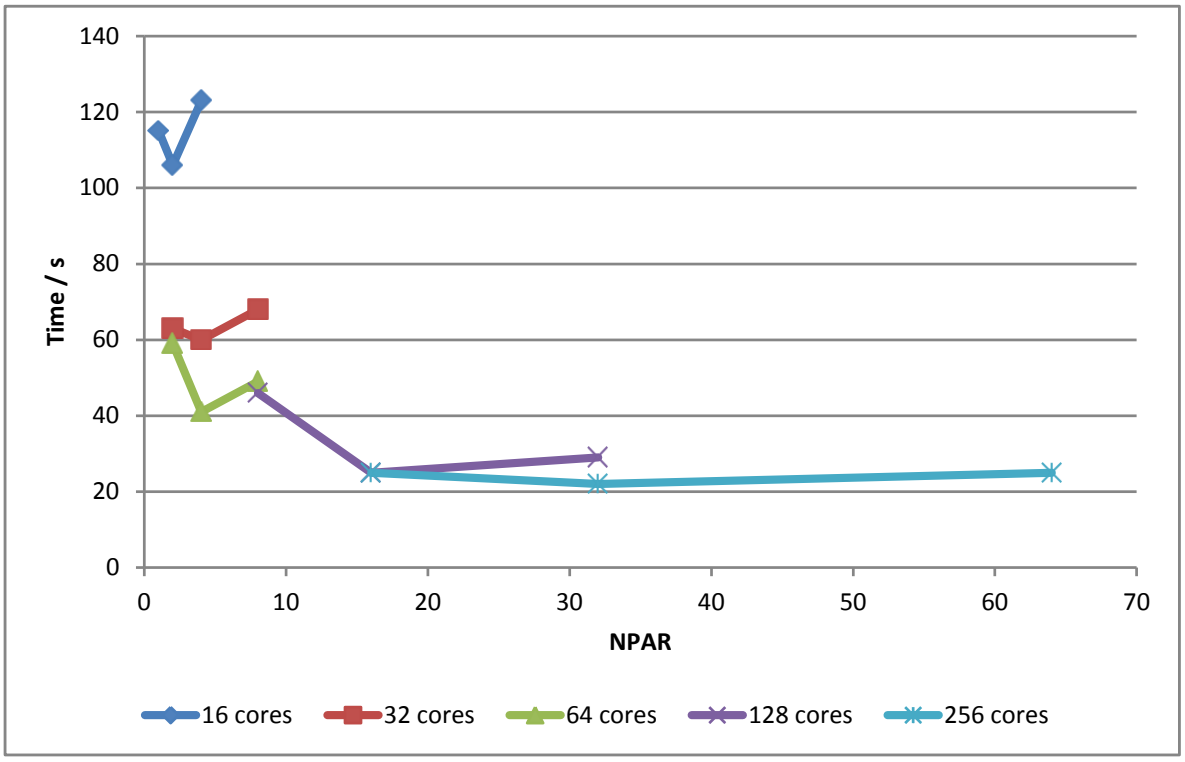

Figure 1: Values of NPAR versus time to solution for various numbers of cores for Bench 1.

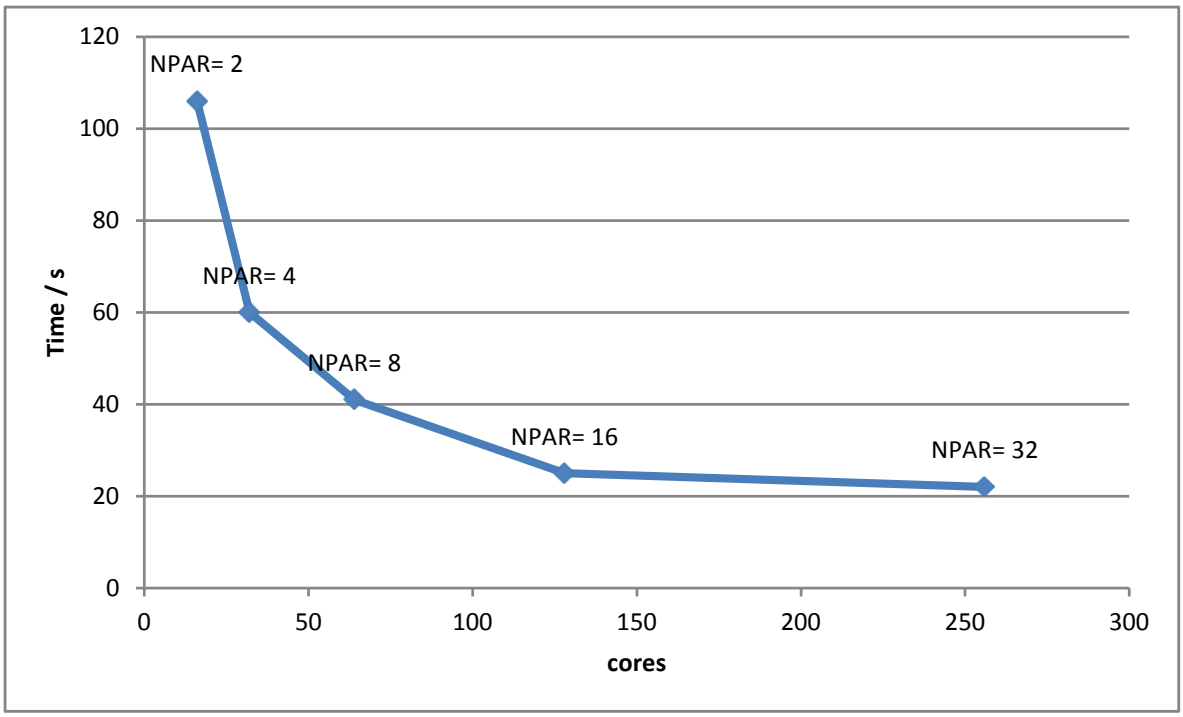

Figure 2: Plot of number of cores versus time to solution for Bench 1. The optimum value of NPAR is indicated for each point.

Bench 2: Li defect in ZnO (Hybrid-DFT)

Γ-point code. For this calculation I would recommend using 64 cores.

Note: you cannot change the value of NPAR for hybrid functional calculations; it is fixed at the number of cores.

Cores	NPAR	Time / s
16	16	1571
32	32	1004
64	64	621
128	128	566
256	256	671

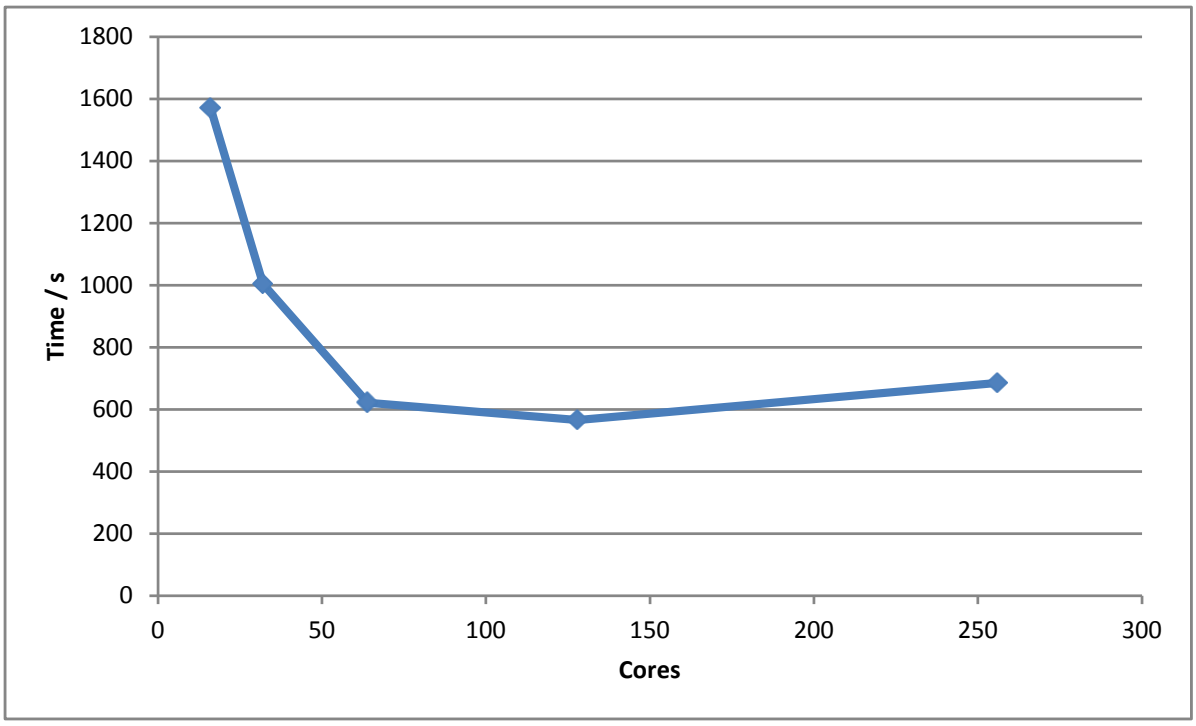

Figure 3: Plot of number of cores versus time to solution for Bench 2.

Bench 3: TiO_2 5×5×5 Supercell

Γ-point code. For this calculation I would recommend using 512 cores and NPAR = 32.

Cores	NPAR	Time / s
128	2	1530
128	4	1435
128	8	1584
128	16	2662
256	8	852
256	16	870
256	32	1423
512	16	624
512	32	572
512	64	850
1024	16	483
1024	32	460
1024	64	475
1024	128	591

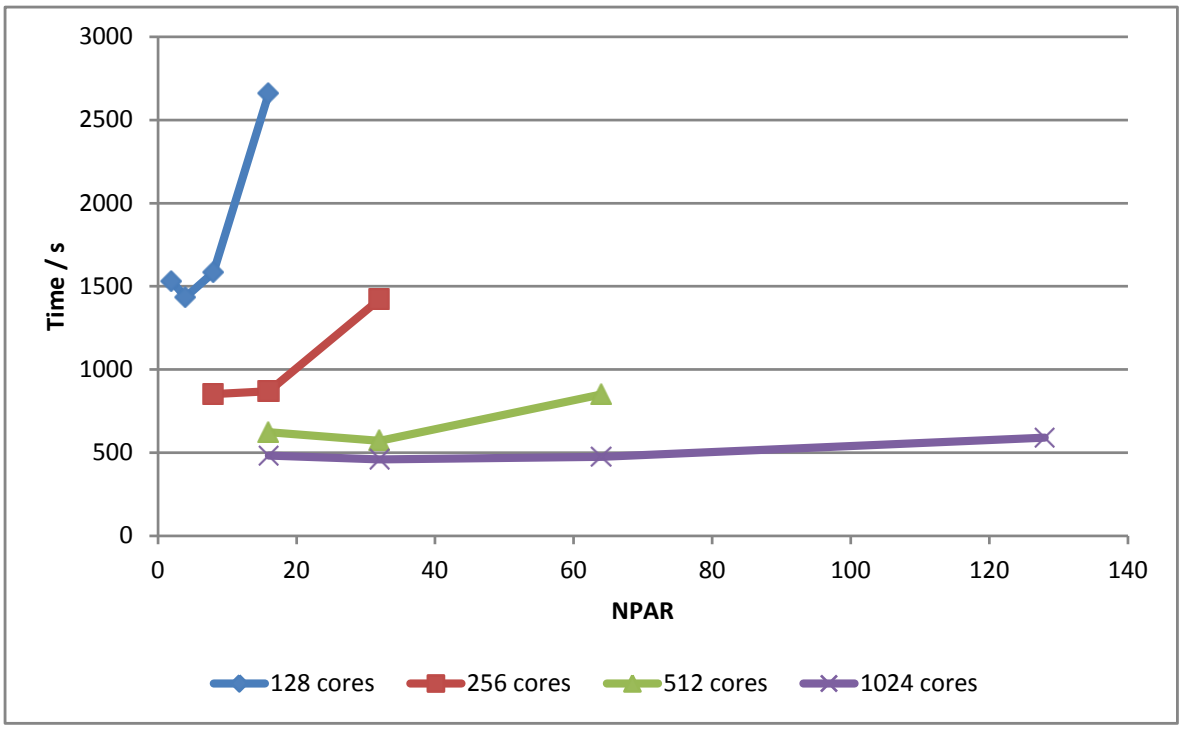

Figure 4: Values of NPAR versus time to solution for various numbers of cores for Bench 3.

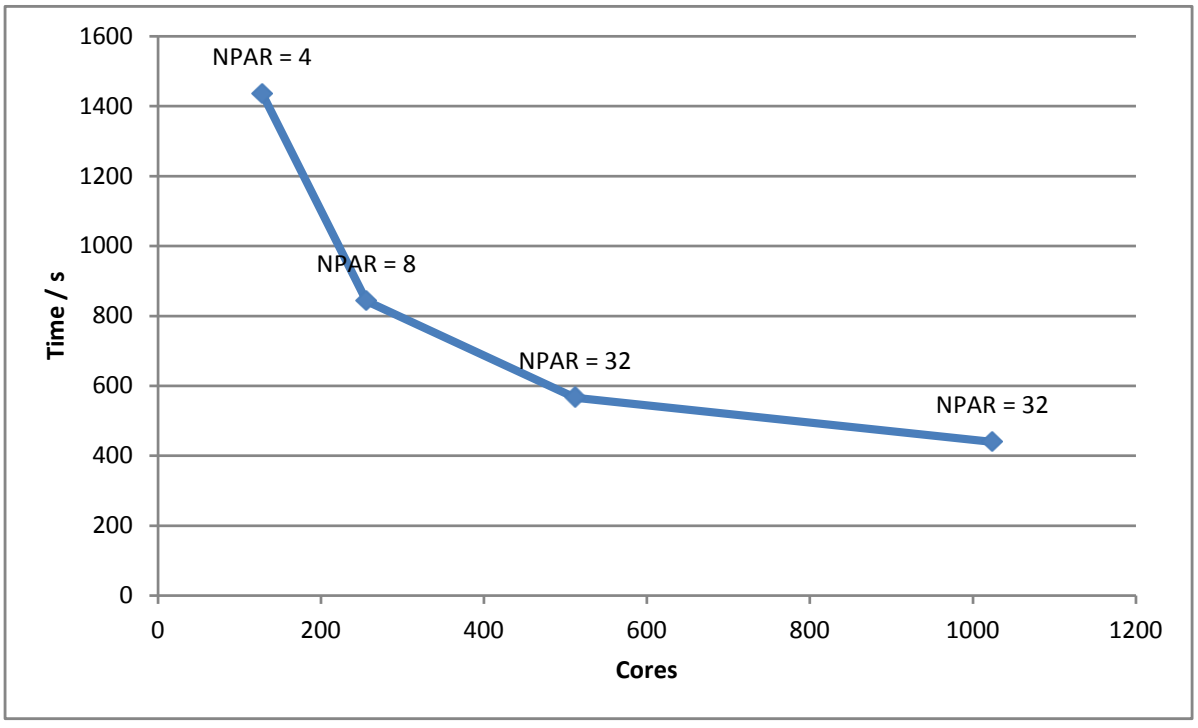

Figure 5: Plot of number of cores versus time to solution for Bench 3. The optimum value of NPAR is indicated for each point.

Summary

- PAW calculations in VASP 5.2 do not scale well when (number of cores) >> (number of atoms) as the PAW calculation is parallelised over number of atoms.
- Value of NPAR depends on size of system you are studying and the number of cores you are running on.

Here are some tentative guidelines for running VASP 5.2 on HECToR efficiently:

- If you can test to find the optimal NPAR value with a single SCF cycle you should do this.
- The more cores you are using the less critical the value of NPAR becomes.
- For the smaller benchmarks (32 and 64 atoms) a good rule of thumb seems to be to choose NPAR = (number of cores) / 8.
- For the larger benchmark (750 atoms) the rules are not so clear cut but a good starting point would be NPAR = (number of cores) / (16 or 32).