

Session 3:

Running VASP in parallel – guidelines and results



"Beskow": Cray XC40 supercomputer at PDC in Stockholm

Guidelines for Beskow

- **Regular DFT:** > need 100 atoms or 400 bands
- **Hybrid DFT:** > 50 atoms or 200 bands
- Use **k-point parallelization** if possible
- Speed per node is **2x-4x of Triolith**
- Use **24 cores per node** instead of 32.

```
#!/bin/bash
#SBATCH -J GAB512
#SBATCH -t 03:00:00
#SBATCH -N 48

aprun -n 1152 -N 24 -S 12 /pdc/vol/vasp/5.3.5-31Mar14/build04/vasp
```

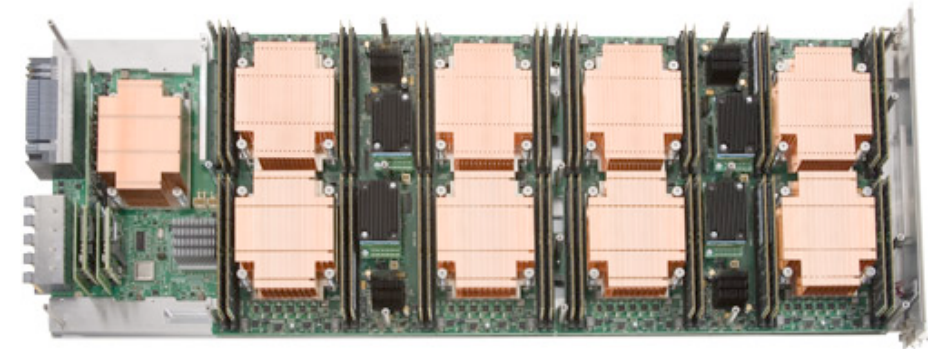
- Beskow has **64 GB memory per node**
- 64GB/24 cores = 2.7 GB/core vs 2 GB/core on Triolith
- Good news for hybrid-DFT/GW etc.

Beskow hardware overview

Compute node

32 cores (Intel Xeon E5v3 2.3 Ghz)
64 GB of DDR4 memory
No local hard disk

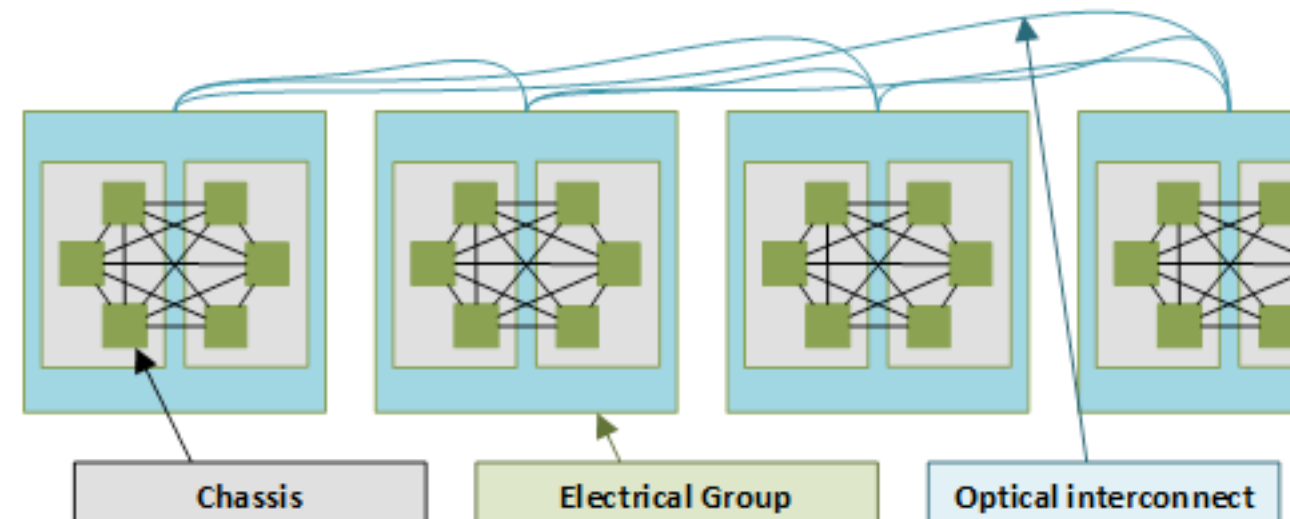
1 blade connects **4 nodes**



1 chassis connects 16 blades = **64 nodes**



6 chassis form a group = **384 nodes**



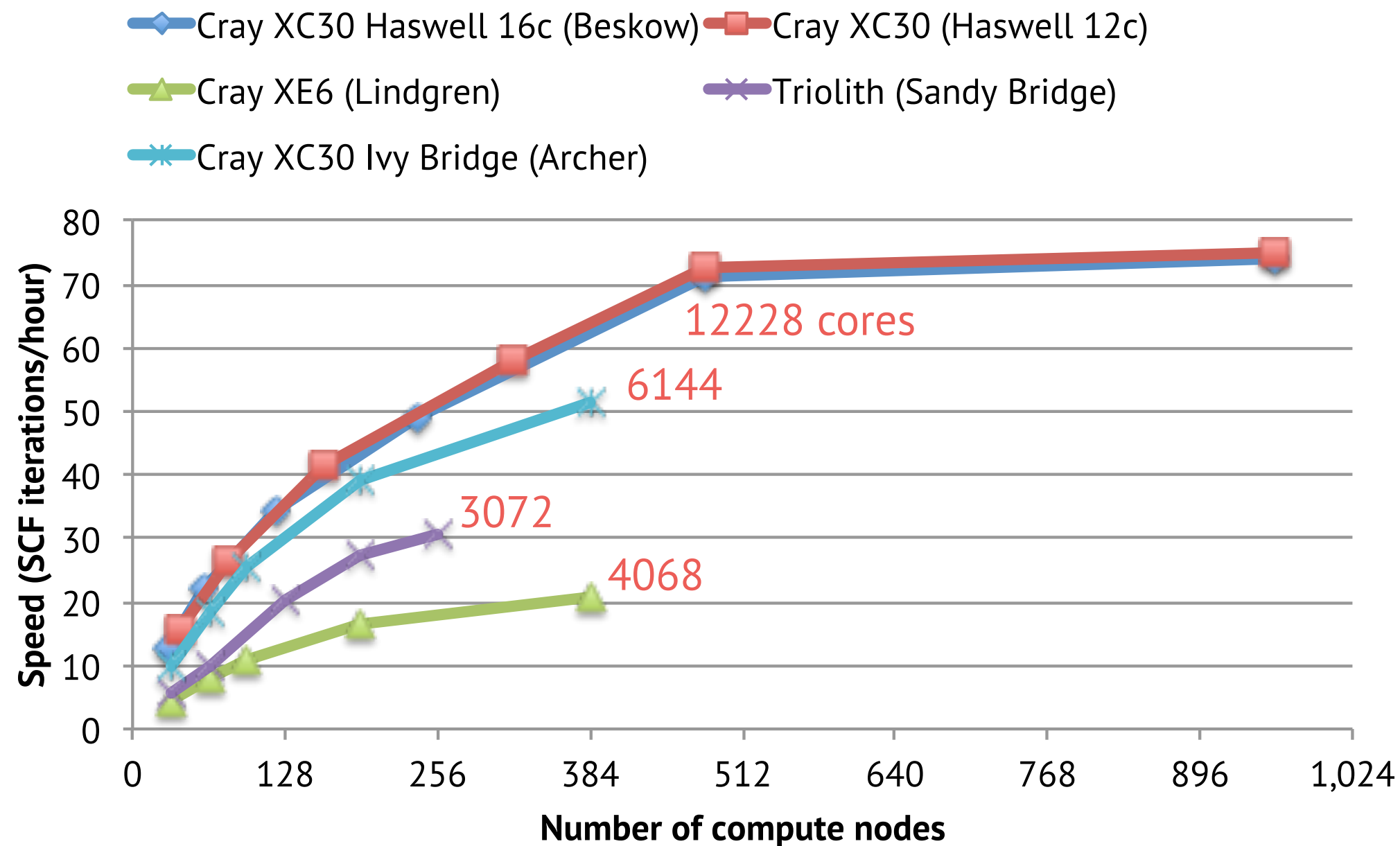
Note: Beskow will run the SLURM queue system (same as Triolith)

In total, **1636 compute nodes** with 52,352 cores



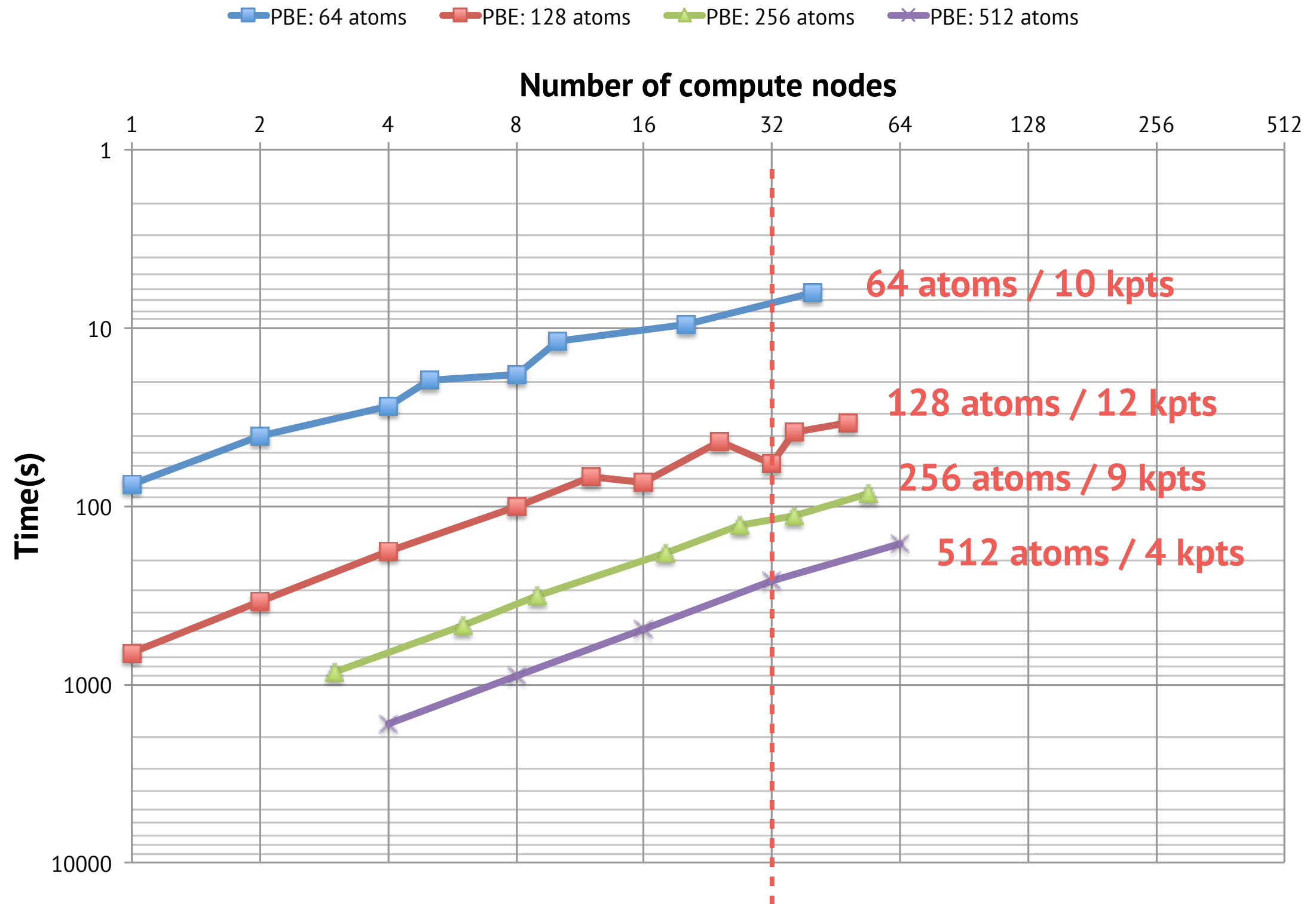
VASP: GaAs supercell (5900 atoms)

Standard DFT calculation



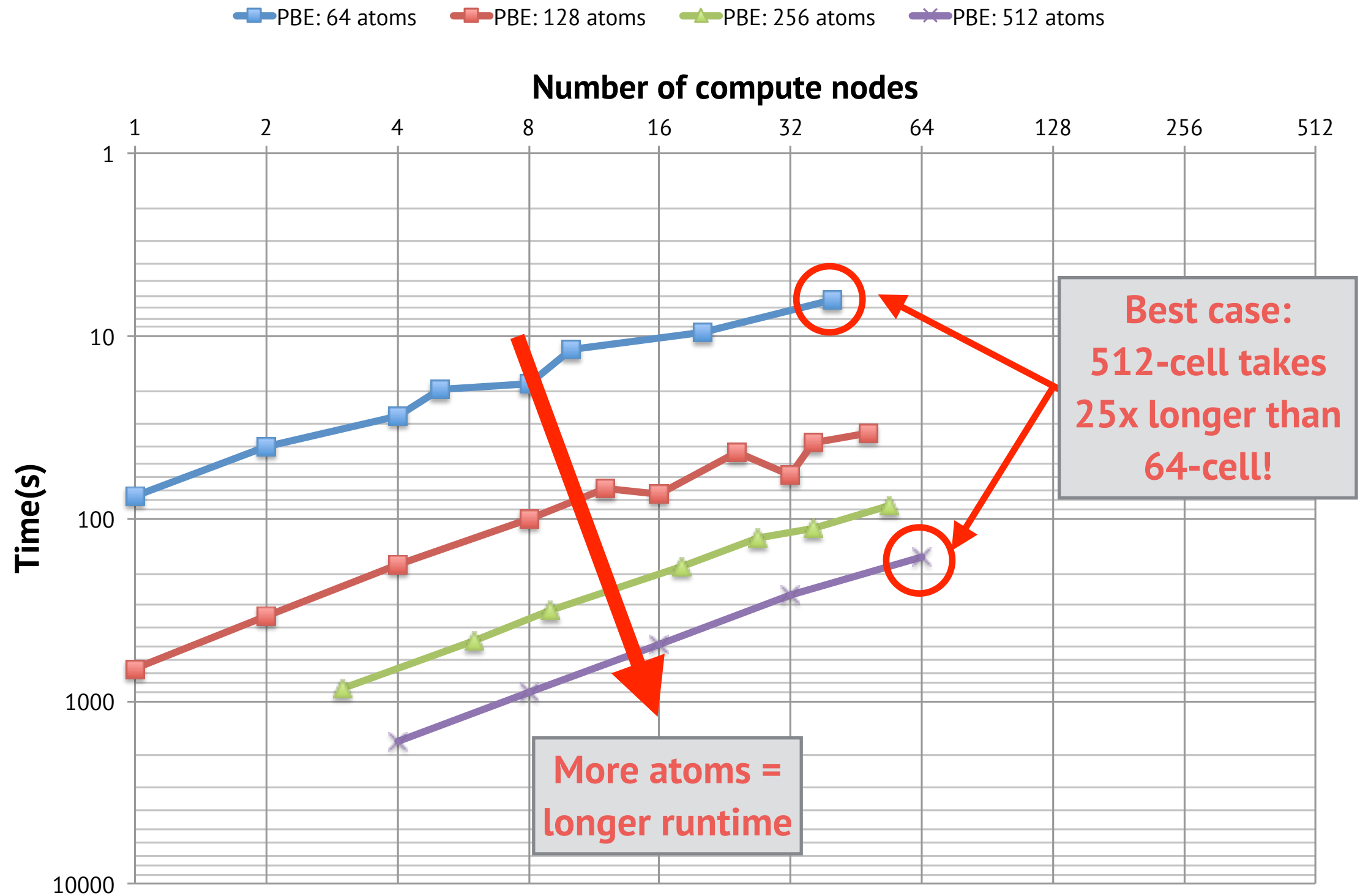
14752 electronic bands, 2 bands/core $\approx$ 7000 cores

GaAsBi supercells on Beskow (DFT-GGA)

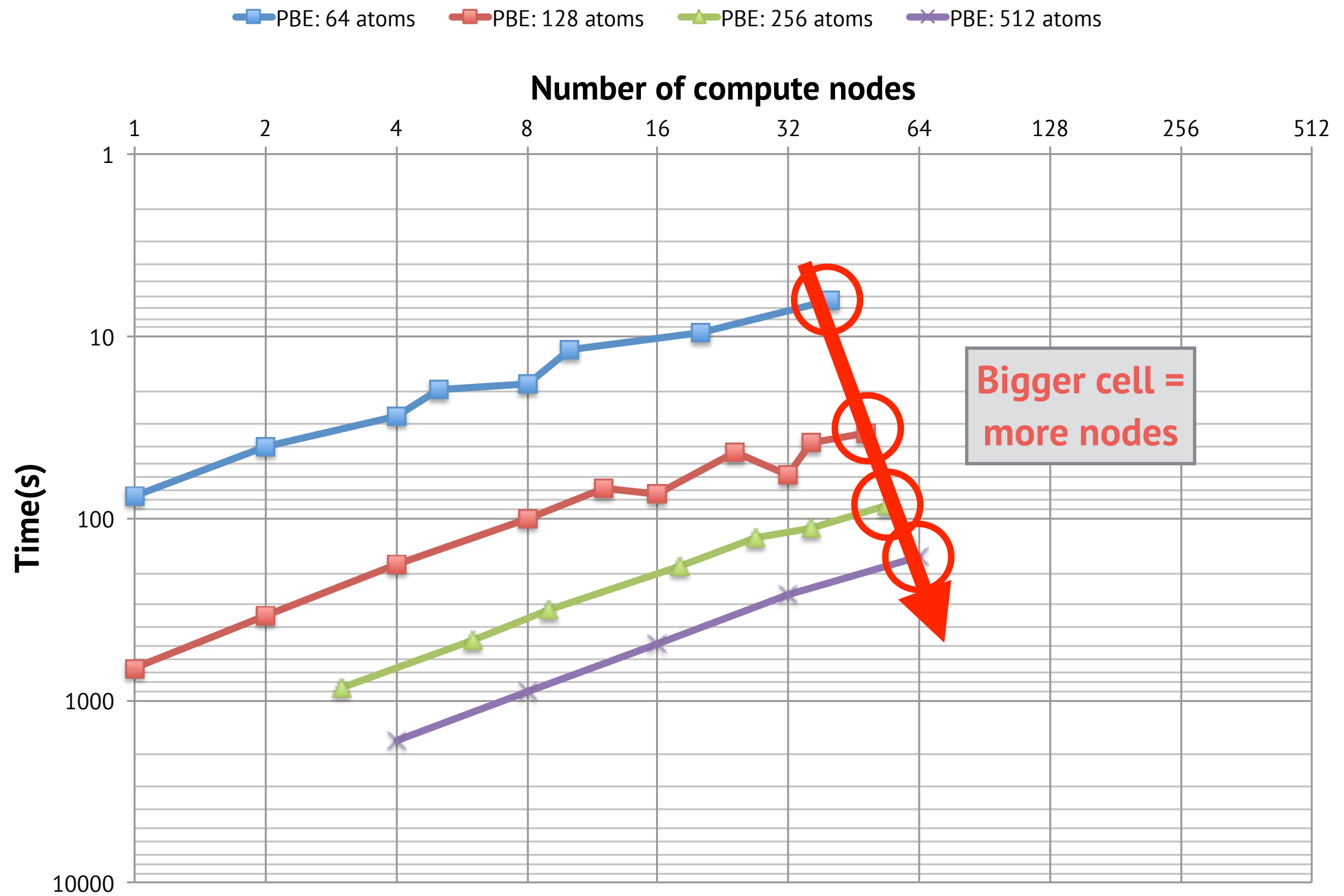


PDC's recommended job size for Beskow
("less than 1024 cores discouraged")

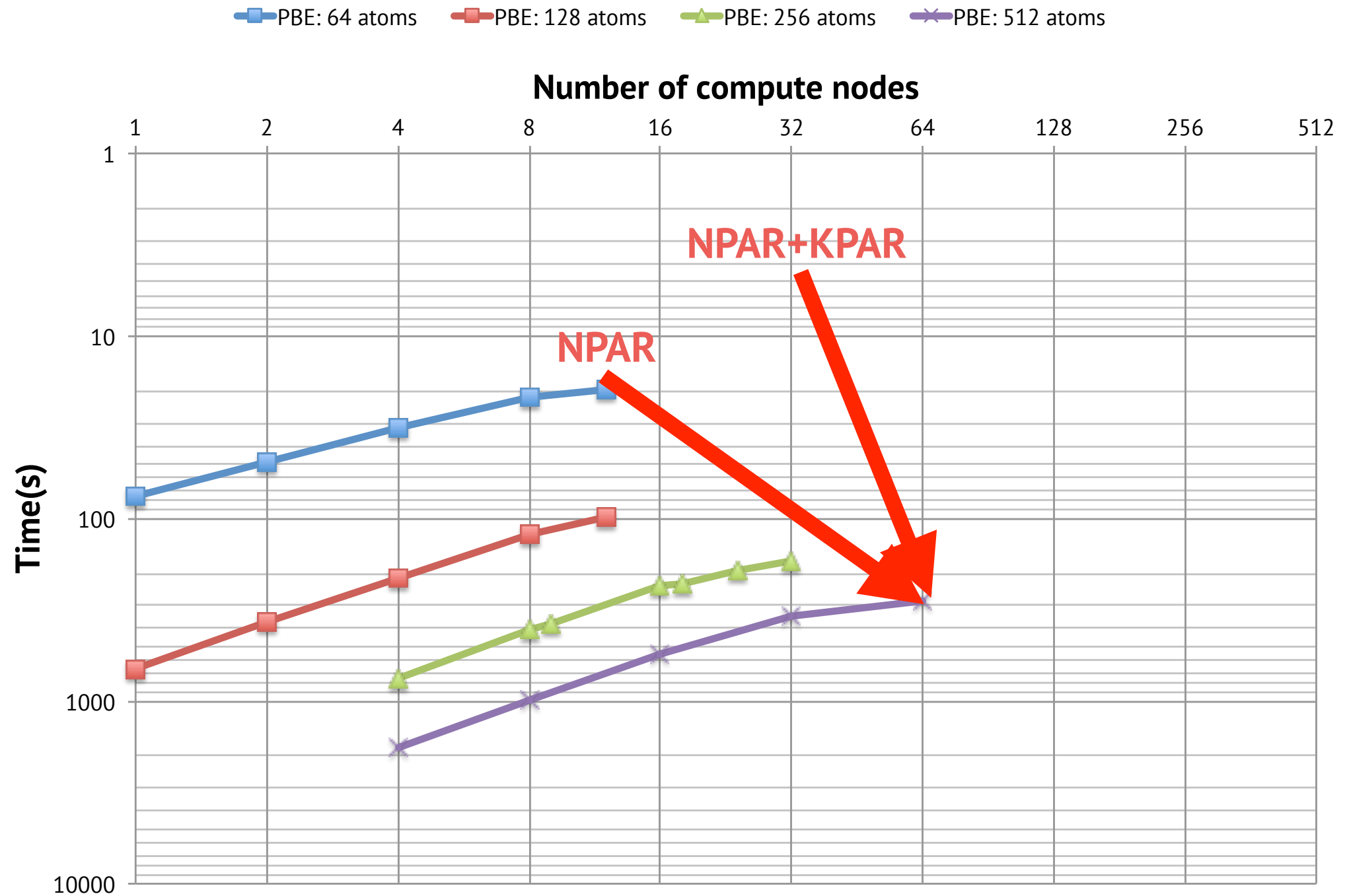
GaAsBi supercells on Beskow (DFT-GGA)



GaAsBi supercells on Beskow (DFT-GGA)



GaAsBi supercells on Beskow (DFT-GGA) no KPAR



64 atoms: 192 bands = 12 nodes * 16 cores/node

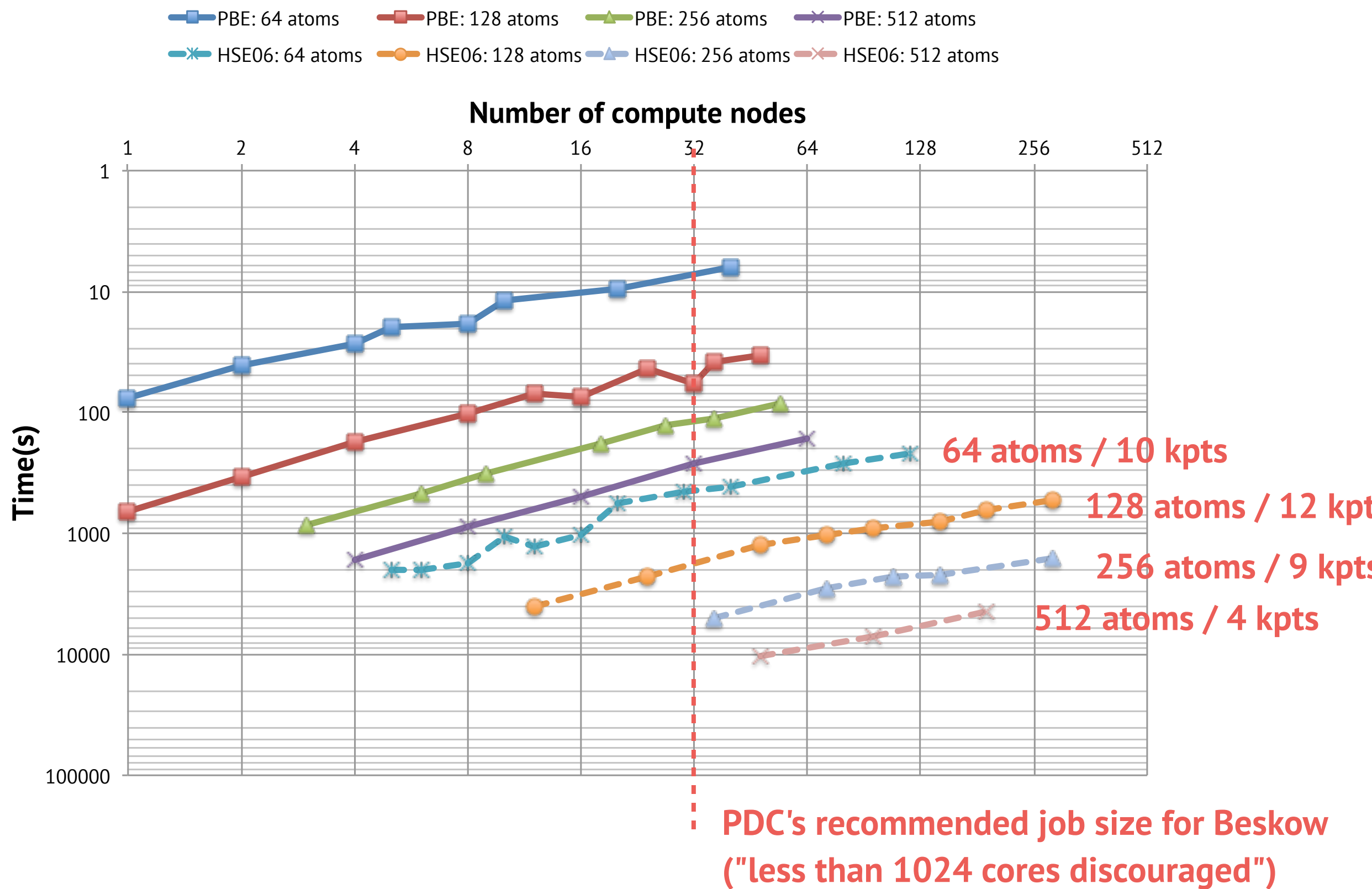
512 atoms: 1536 bands = 64 nodes * 24 cores/node

Summary: How many compute nodes on Beskow?

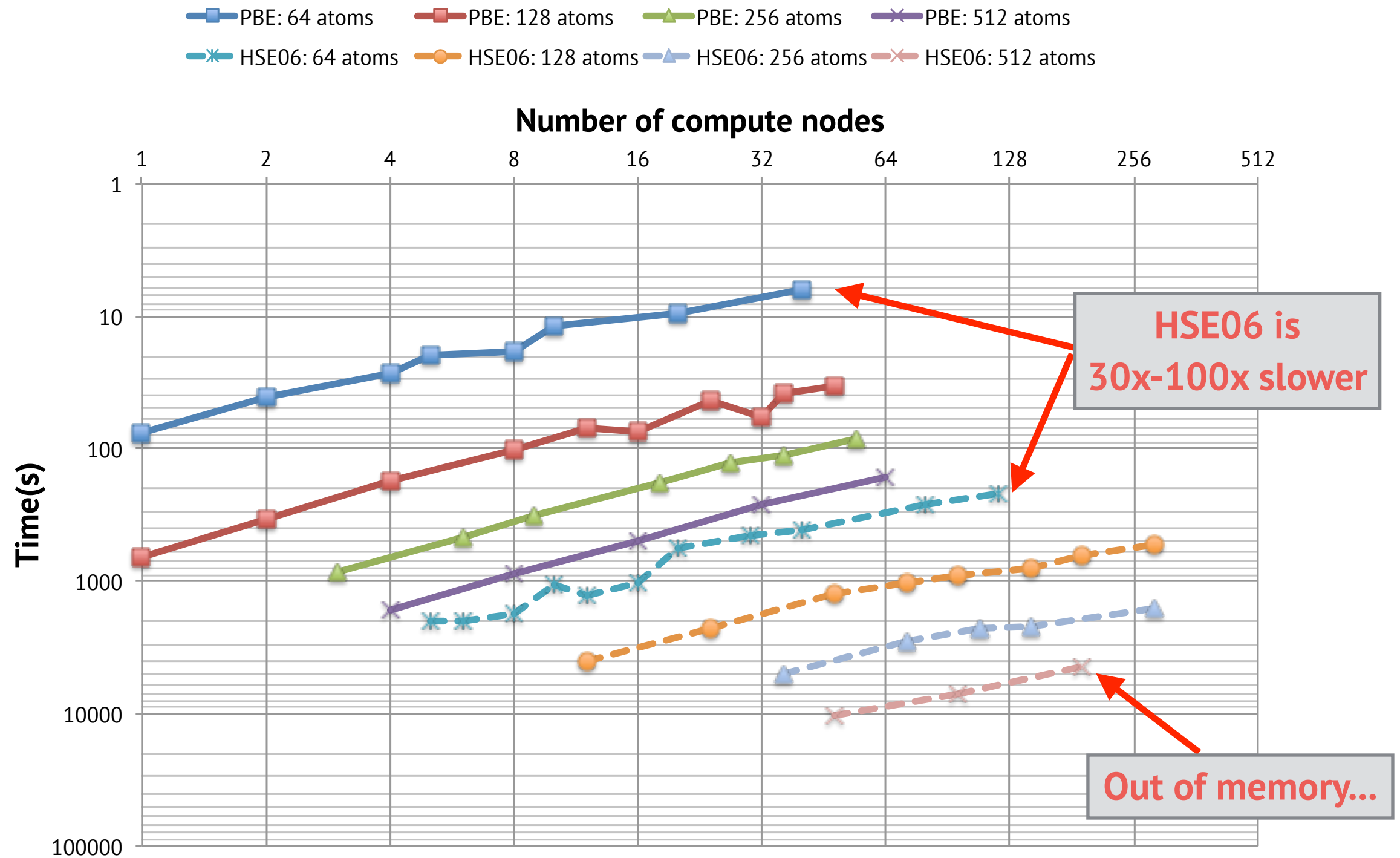
Size of cell	Without KPAR	KPAR
64 atoms	4	10
128 atoms	12	24
256 atoms	32	54
512 atoms	32	64

K-point parallelization ("KPAR") let's you double the number of nodes.

GaAsBi supercells on Beskow (HSE06 DFT-hybrid)

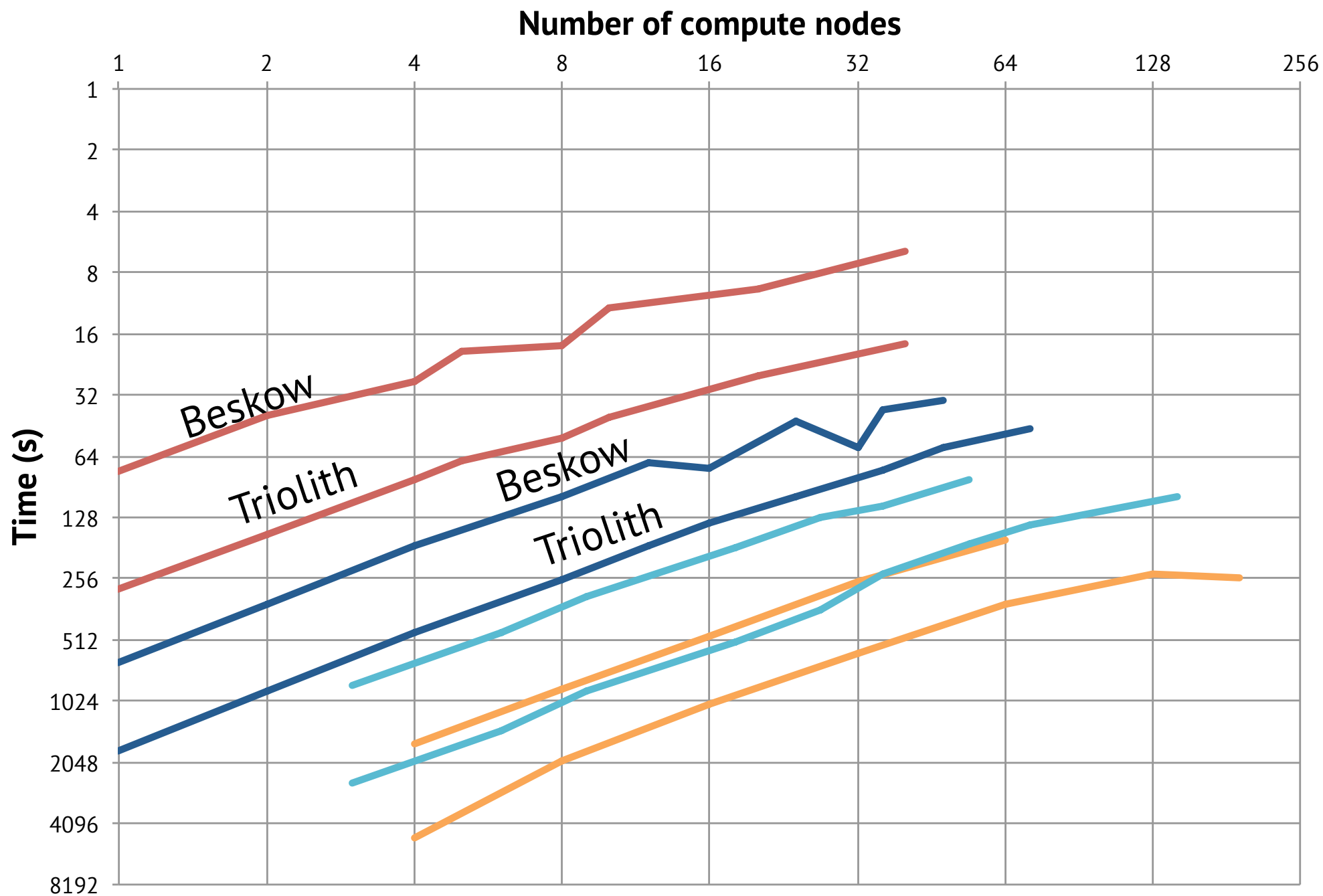


GaAsBi supercells on Beskow (HSE06 DFT-hybrid)



Adding compute nodes will never make HSE06 as fast as GGA

GaAsBi supercells: Beskow vs Triolith (DFT-GGA)



Beskow is 2-4x faster per compute node

*VASP does not benefit from the fast network on the Cray.
(Parallel scaling is same – or even worse)*