Specialist course on efficient use of VASP

(and other electronic structure codes
on modern supercomputers)

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More info at the web page:
http://www.nsc.liu.se/~pla

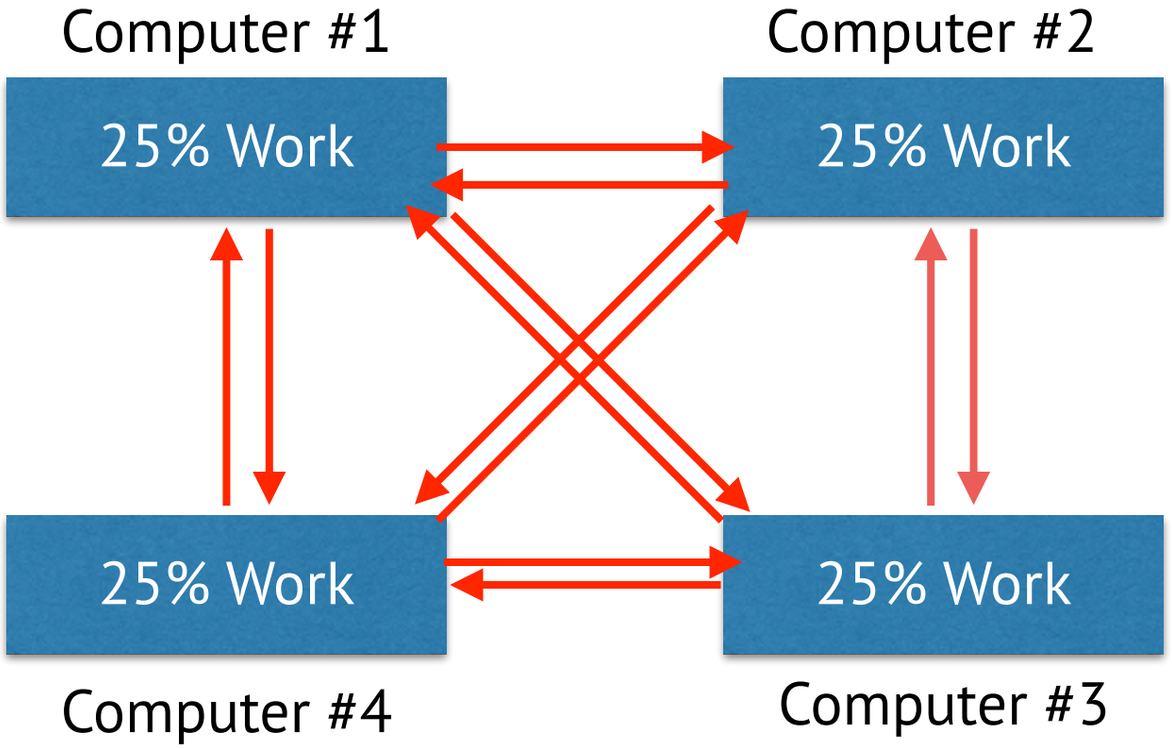
Electronic structure software packages

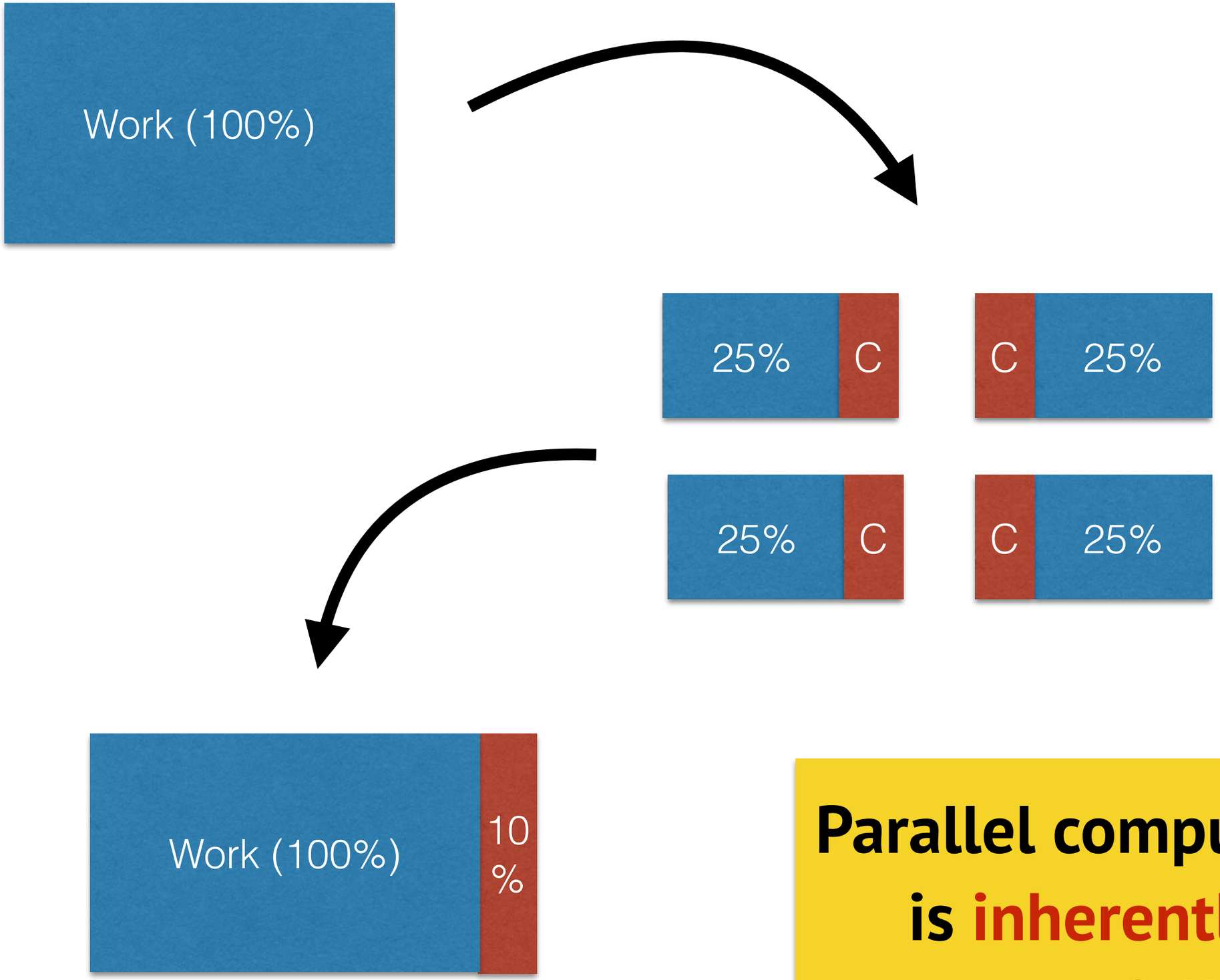
General performance aspects

- http://www.psi-k.org/codes.shtml

What happens in a parallel program?

Work (100%)



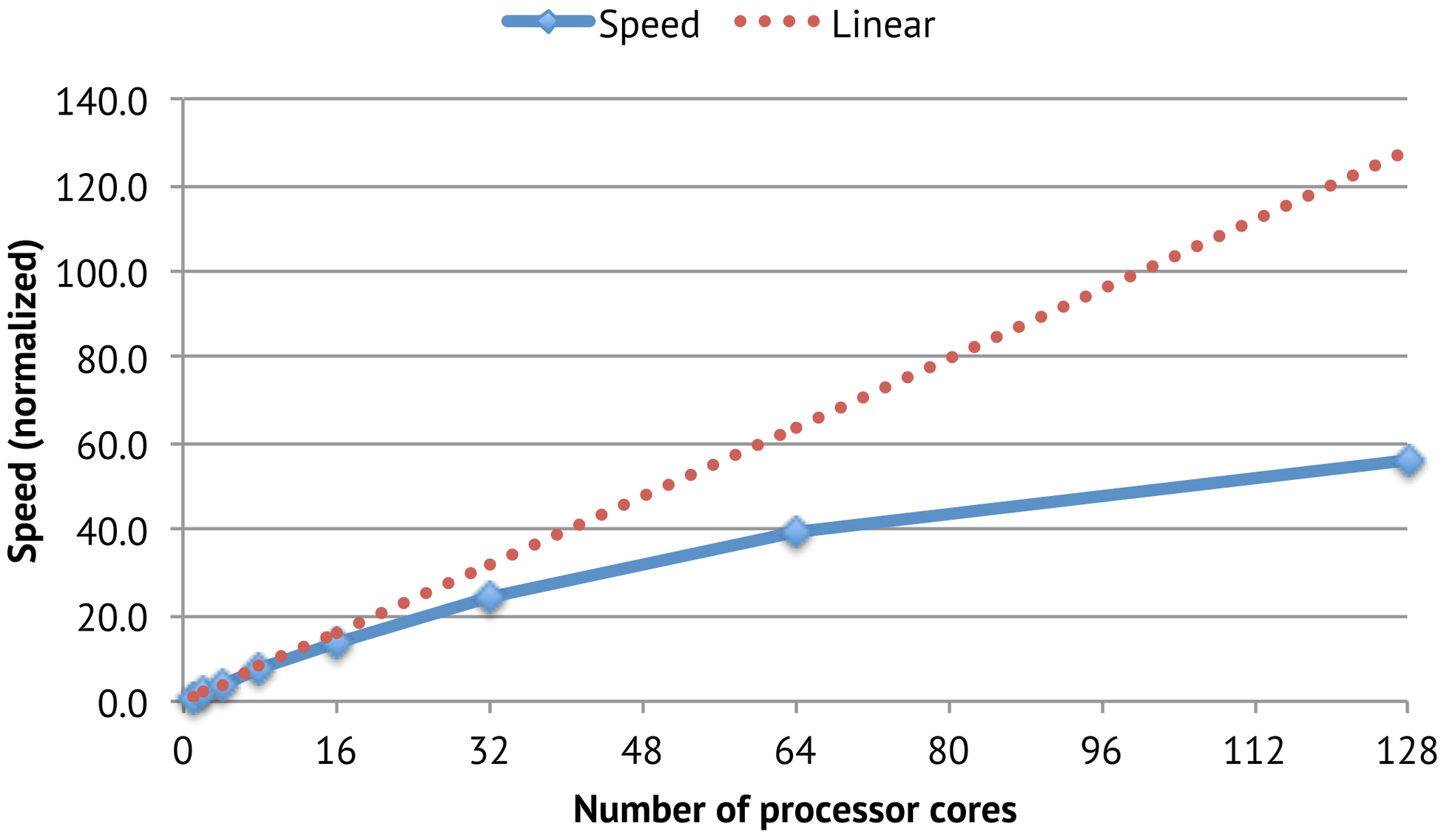


Parallel computing is inherently wasteful!

$$Speed(n) = \frac{1}{S + \frac{1}{n}(1 - S)}$$

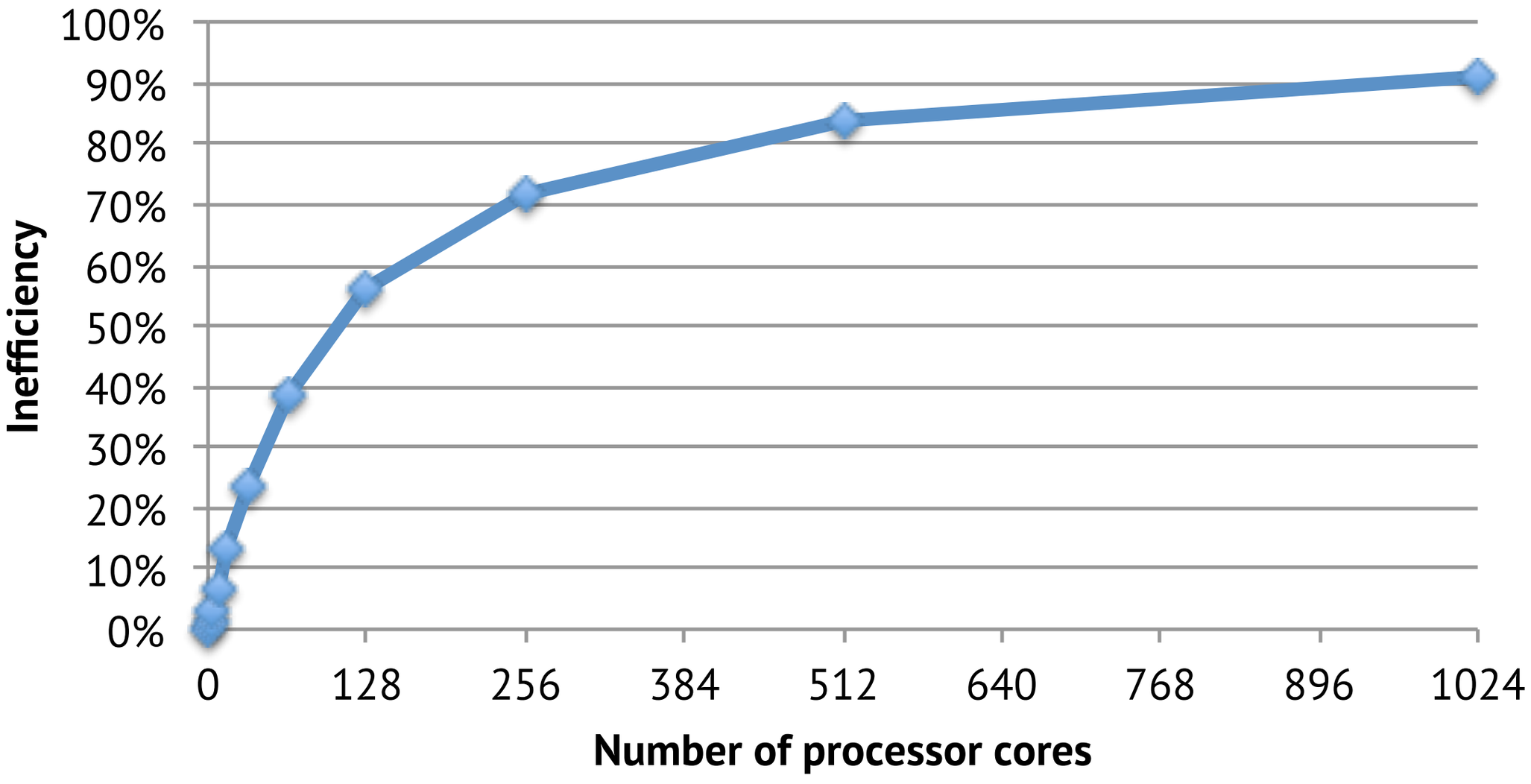
Parallel speed-up according to Amdahl's law

(Program is 99% parallel!)



Wasted computer time vs parallel job size

(Program is 99% parallel)



Dear Professor N.N.,

We regret to inform you that we have decided to cut your time allocation from 1000 node days to 500 node days.

Best regards,
Computer Center Staff

“Mechanical Sympathy”

– Hardware and software working together in harmony

Magic numbers

Use 24 or 25 compute nodes?

511 vs 512 bands (or grid points)?

You have 4 compute nodes: 4 or 5 k-points in Brillouin zone?

Magic numbers

Use 24 or 25 compute nodes?

24 servers are connected to 1 Infiniband network switch

511 vs 512 bands (or grid points)?

511 = 7 x 73

whereas 512 = 2^9

You have 4 compute nodes: 4 or 5 k-points in Brillouin zone?

4 (with parallelization over k-points)

Post lecture remark *regarding power-of-two numbers such as 512. These numbers are nice for load-balancing at a high hardware level (nodes, NUMA zones, processors). At a low level, inside a subroutine, odd numbers such as 513 can actually be better to use because it potentially minimizes memory cache misses.*

Memory issues

The #1 cause of a crashing DFT calculations is
running out of memory
(Especially for DFT-HF-hybrid or GW)

A simple non-linear example:
Increase 2x2x2 k-point grid to 4x4x4 grid.
How much more memory is needed?

Memory issues

Example 2:

Increase the plane-wave basis set from 400 eV to 600 eV

How much more memory is needed?

Memory issues

Example 2:

Increase the plane-wave basis set from 400 eV to 600 eV

How much more memory is needed?

$$n_{pw} \propto \texttt{cut-off}^{\frac{3}{2}}$$

So memory usage increases ca 1.8x

Distributing memory

1 node

Memory footprint

4 compute nodes

Copy 1 (110%)

Copy 2 (110%)

Copy 3 (110%)

Copy 4 (110%)

35% mem

35% mem

35% mem

35% mem

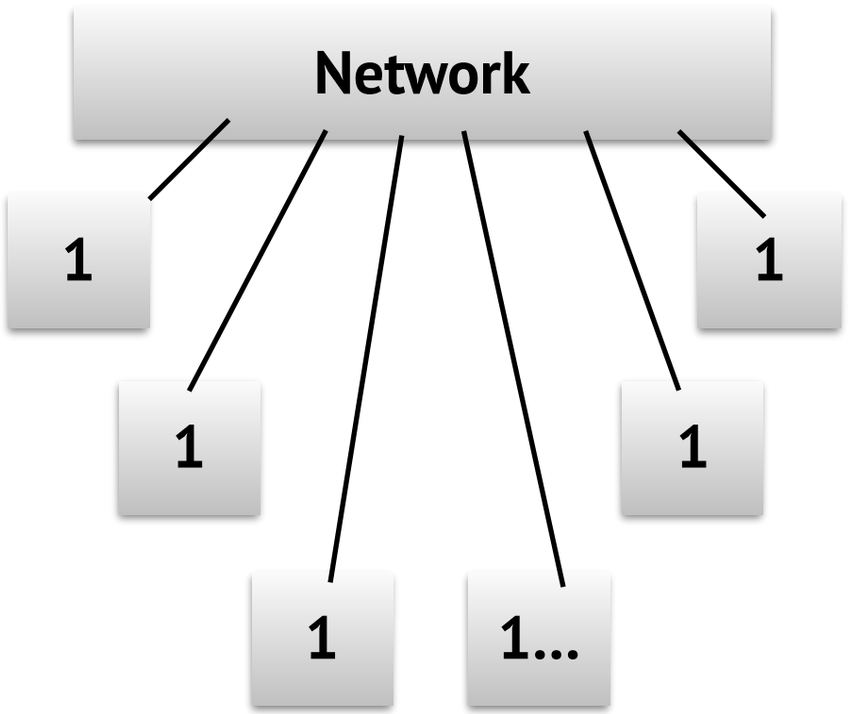
Memory demands can decrease (or increase!) by the number of processors used.

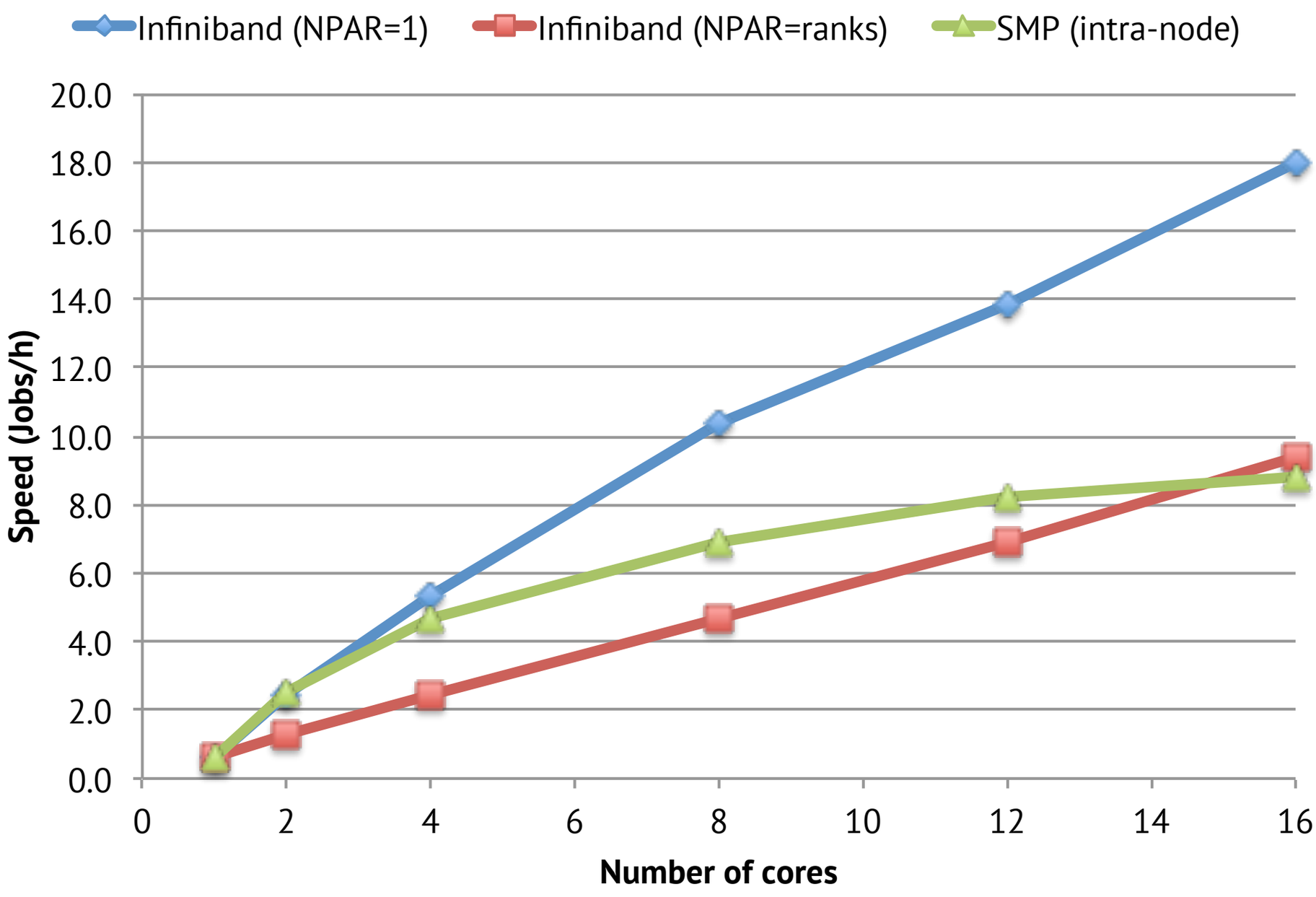
Bottlenecks

1. **Total memory bandwidth**
2. Network latency
3. Network bandwidth
4. Number of cores
5. Clock frequency

What is faster?

16 compute nodes using 1 processor (2.2 Ghz) connected with Infiniband



1 node using 16 processors (2.6 Ghz)

VASP scaling: Shared-memory vs Infiniband