



HPC for Life Sciences at University of Innsbruck

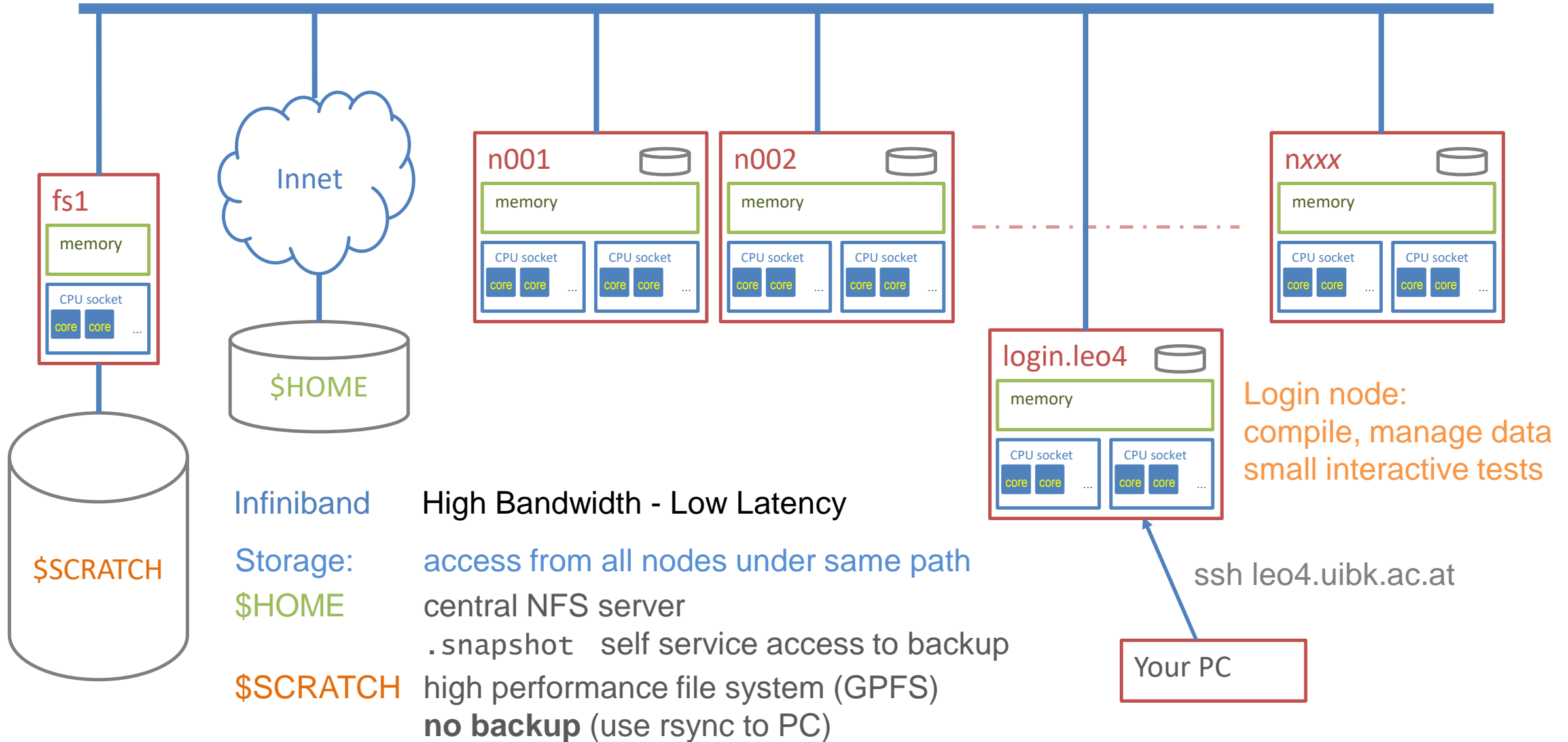
Hermann Schwärzler

IT Services (ZID)

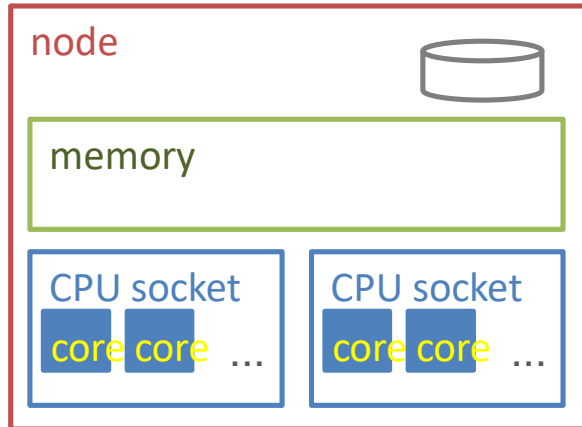
- HPC-Systems of Research Area Scientific Computing
 - Leos (Compute Clusters)
 - Mach2 (Shared Memory Server) @JKU Linz
- Why HPC (Examples)
- Software

Compute Cluster - Leo3, Leo3e and Leo4

IB (Infiniband Network)



Compute Clusters Leo3, Leo3e and Leo4



OS (Linux)

nodes

CPU-Cores / Node

Memory / Node

Leo3

CentOS 6

≤ 162 (legacy)

12

24 GB

Leo3e

CentOS 7

45

20

43 × 64 GB
2 × 512 GB

Leo4

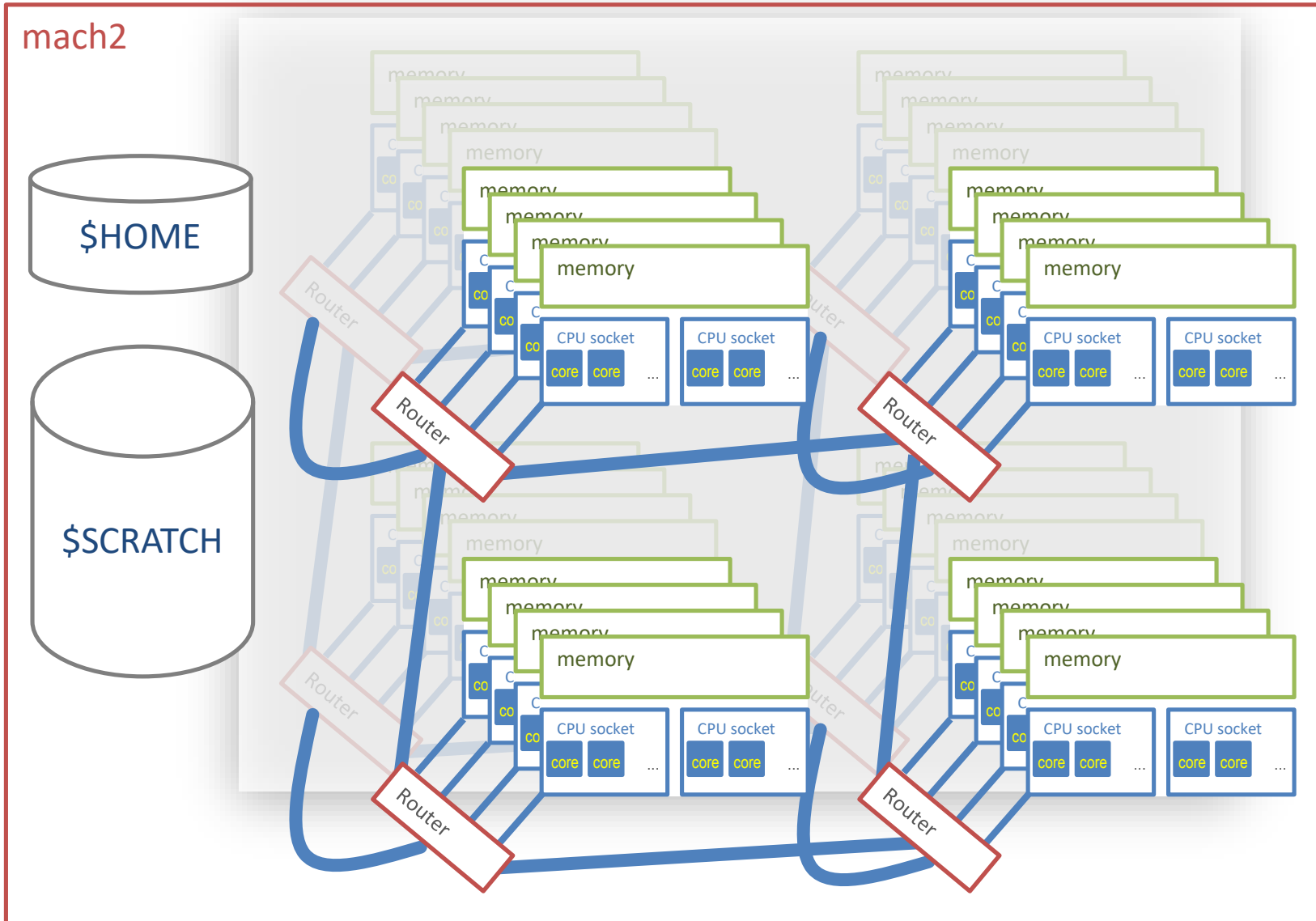
CentOS 7

48 + 1 (with 4 GPUs)

28

44 × 64 GB
4 × 512 GB
1 × 384 GB (GPU)

Shared Memory Server - Mach2



72 blades (“nodes”)

- 24 CPU cores each
- 64 x 256 GB + 8 x 512 GB

Fast Interconnect between all blades.

For OS and Software:
Single machine

- 1728 CPU Cores
- 20 TB Memory

ssh mach2.uibk.ac.at

Your PC

What HPC makes possible (examples):

Capability Computing

Run **large** task on **big machine** – virtually impossible on small machine

Examples:

- De novo assembly with e.g. *trinity*: terabytes of RAM
 - -> Mach2
- Using *NCBI BLAST* for querying NCBI databases *nr* or *nt*: 100 to >200 Gigabytes of RAM
 - -> Bigmem-nodes on Leo3e or Leo4

Capacity Computing

Run **many small tasks** in less time - possible but “would take forever” on small machine

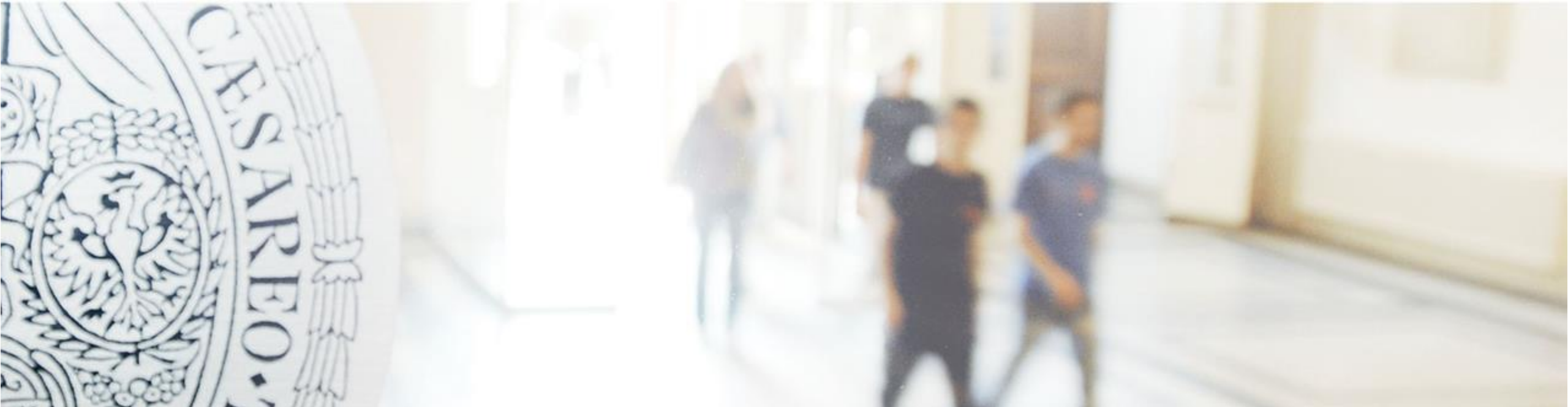
Example:

- Find correct/optimal value for *k* with *structure* (a program for inferring population structures) might need e.g. 100 runs of 10 hours each:
 - 6 weeks when run sequentially
 - Probably a weekend (or less) on Leo3e or Leo4

- Any Software that runs on Linux.
- Self-installation (in scratch area) possible.

Installed by us (as of today):

```
----- /usr/site/hpc/modules/leo4/Bioinformatics -----  
BioPerl/1.7.2      cutadapt/1.18      mothur/1.41.3      stacks/2.2  
Bioconductor/3.8  dadi/2.0.3         mummer/3.23        stacks/2.3b  
HOMER/4.10        deeptools/3.2.1    mummer/4.0.0beta2  structure/2.3.4  
HTSeq/0.11.1      fastqc/0.11.8      ncbi-blast/2.7.1+  trim_galore/0.6.1  
NextGenMap/0.5.5  gatk/3.8-1         ncbi-blast/2.8.1+  usearch/11.0.667  
RSEM/1.3.1        gatk/4.0.12.0     pear/0.9.2         vcftools/0.1.16  
RnBeads/2.0.1     illumina2bam/1.19  picard/2.18.23     vsearch/2.13.4  
STAR/2.7.0f       iqtree/1.6.12      pmerge/1.0  
admixture/1.3.0   mothur/1.39.5      samtools/1.9
```



Thank you!