Practical Introduction to UL HPC

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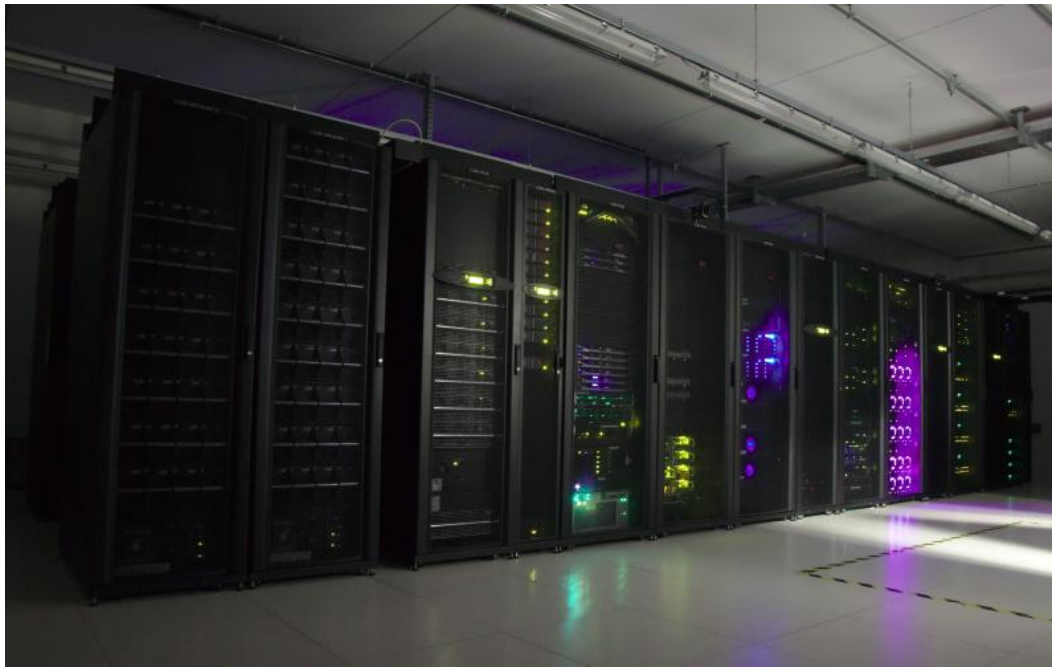
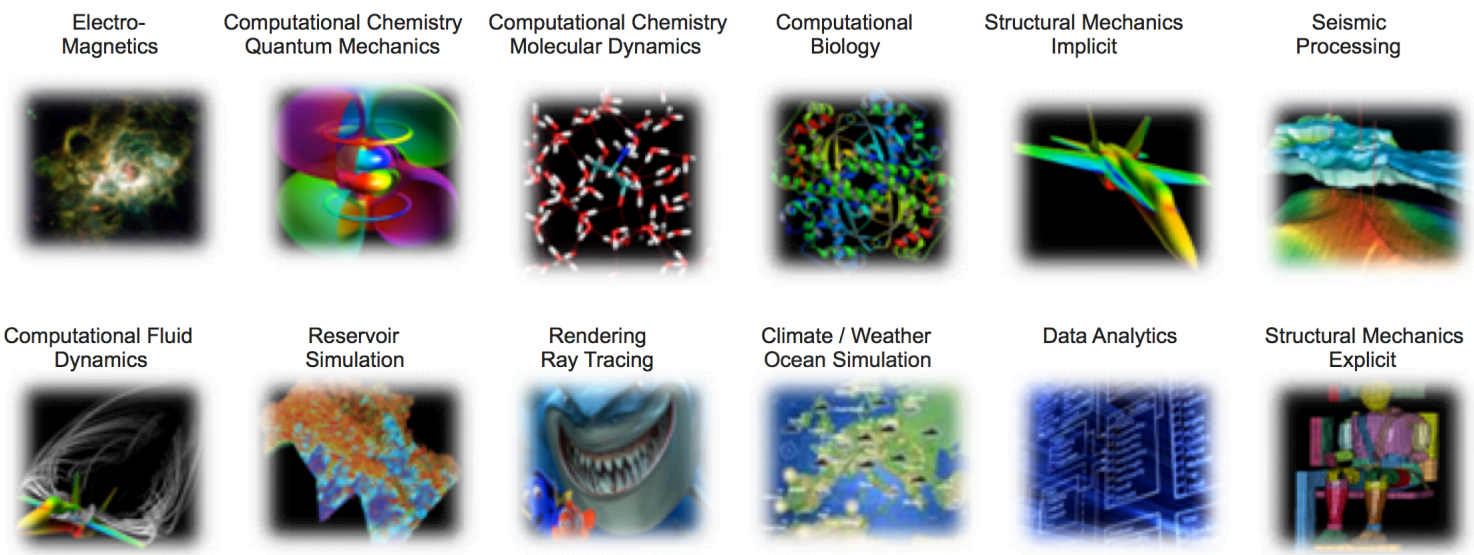
UL HPC School
June 25, 2015



Outline

Computer Simulation is everywhere



- Computational Fluid Dynamics (OpenFOAM)
- Finite Element Analysis (Abaqus)
- Climate / Weather / Ocean Simulation (WRF)
- Molecular Dynamics (Gromacs, Amber)
- Quantum Chemistry (Quantum Espresso)
- Visualization (Paraview)
- Data processing (R, Matlab)
- ...

What is High Performance Computing?

High Performance Computing (HPC)

- Use of parallel and distributed computers with fast interconnects
- To execute an application quickly and efficiently

Why parallel computers?

- Performance of single CPU core is getting limited (power, physics)
- Multiple cores are used to increase the computing capacity

HPC is challenging

- Active research domain
- Provides tools for many other researchers

Can you benefit from HPC?

Your application is limited by the performance of your computer

	Your workstation	UL HPC platform[1]
CPU	160 **G**Flops	49.9 **T**Flops
Memory	16 **G**Bytes	20.6 **T**Bytes
Storage	2 **T**Bytes	3.4 **P**Bytes
Network	Ethernet 1 Gb/s	Infiniband 40 Gb/s
Accelerators	1 GPU	29 GPUs

⇒ HPC provides the **tools** for your application to run faster

[1] shared among many users

Other benefits of using the UL HPC platform

over using your personal computer

Long uptime and stable

- Cluster nodes are always running

Remote access

- Start a job from work, check results from home

No administration

- The HPC team maintain the hardware/software

Large software collection

- Scientific and general-purpose applications pre-installed

Backup

- Automatic backup of your Home directory[2]

[2] Always keep a backup of your critical data!

Outline

Know the basics!

Get an account

- `https://hpc.uni.lu/users/get_an_account.html`
- Please read carefully the Acceptable Use Policy

Access the clusters, access and reserve nodes

- Use SSH and public key authentication
  `https://hpc.uni.lu/users/docs/access.html`
- Learn how to use the OAR resource manager
  `https://hpc.uni.lu/users/docs/oar.html`

Transfer files between your computer and the clusters

- Learn how to use tools like `scp`, `rsync`, etc.
  `https://hpc.uni.lu/users/docs/filetransfer.html`

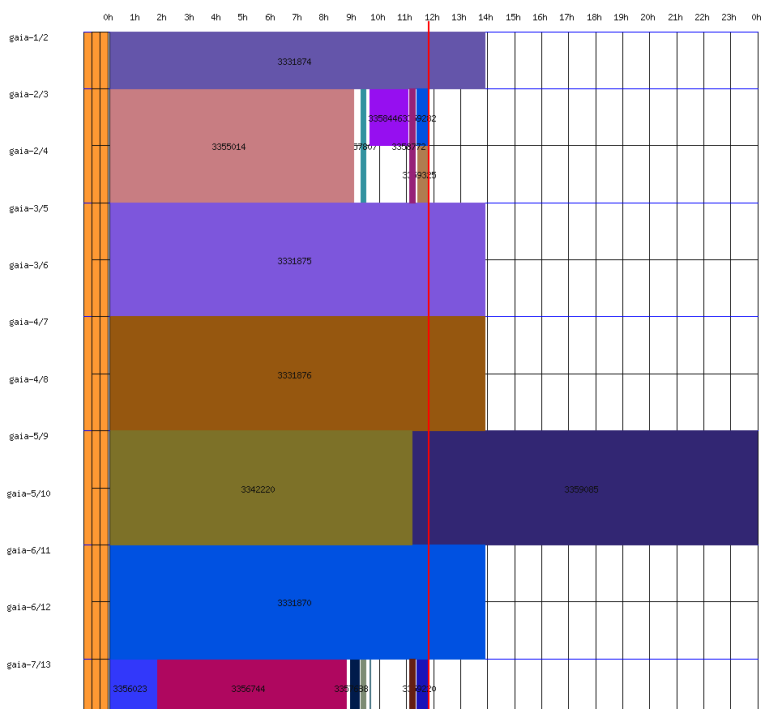
Use pre-installed software

- Search and use software with the `module` command
  `https://hpc.uni.lu/users/docs/modules.html`

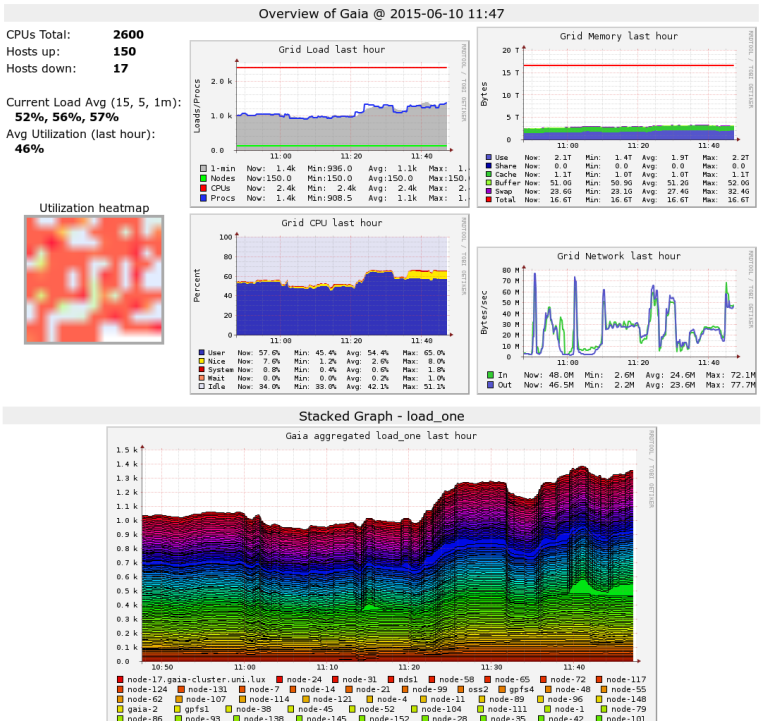
Join session PS 1B to learn the basics!

Check Live Status of the platform

- Current node status with Monika
  `https://hpc.uni.lu/status/monika.html`
- Platform occupation – Gantt chart with DrawGantt
  `https://hpc.uni.lu/status/drawgantt.html`
- Resource usage with Ganglia
  `https://hpc.uni.lu/status/ganglia.html`



DrawGantt



Ganglia

Getting help

- Check the UL HPC quick reference
  `https://hpc.uni.lu/download/documents/ulhpc-quickref.pdf`
- RTFM! Online Documentation available at
  `https://hpc.uni.lu/users/docs/`
- Google is your friend!
- Ask other users on the mailing list `hpc-users@uni.lu`
- Ask the HPC sys-admins `hpc-sysadmins@uni.lu`

Workflow for Experiment Campaigns

1. Before the campaign

- Send data to the clusters
- Check/Install required software

2. Preparation

- Test and debug
- Prepare launcher script

3. Execution

- Run the campaign
- Monitor the execution

4. After a campaign

- Retrieve output data
- Archive and cleanup your data

Workflow for Experiment Campaigns

1. Before the campaign → *cf* the Basics

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4. After a campaign → *cf* the Basics

- Retrieve output data
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Experiment campaign: Preparation

Goals

- Make sure everything will run OK
- Prepare submission script / launcher

Interactive approach

- Use option `-I` (Interactive) of `oarsub` command
- Allows to try commands one by one
- Work on a small case with a small number of cores
- Debug and check the results

Why prepare a submission script?

- Contains all commands and parameters
  $\Rightarrow$ Easy re-execution
- No need to stay in front your computer

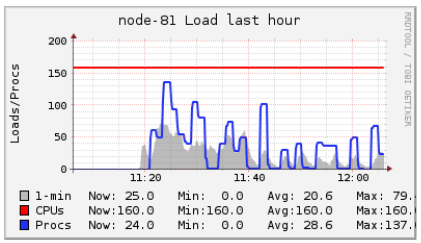
Experiment campaign: Execution

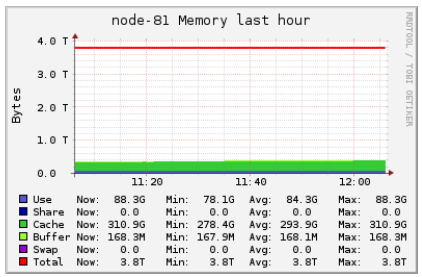
Submit the jobs

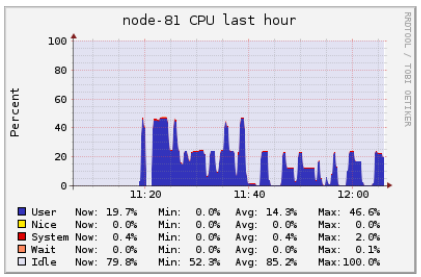
- Use the submission script / launcher
- Submit to OAR with option `-S` (Script) of `oarsub`
- Actual experiment execution with possibly many nodes
- Non interactive execution, it might not start immediately

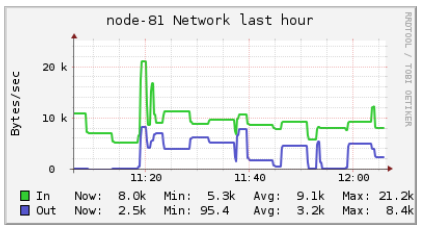
Monitor the execution

- Status of your job: `oarstat -j <OAR_JOBID> -f`
- Output/Logfile of your application
- Resource usage (CPU, memory, etc.)
  on the node: `htop`
  with Ganglia: `https://hpc.uni.lu/status/ganglia.html`









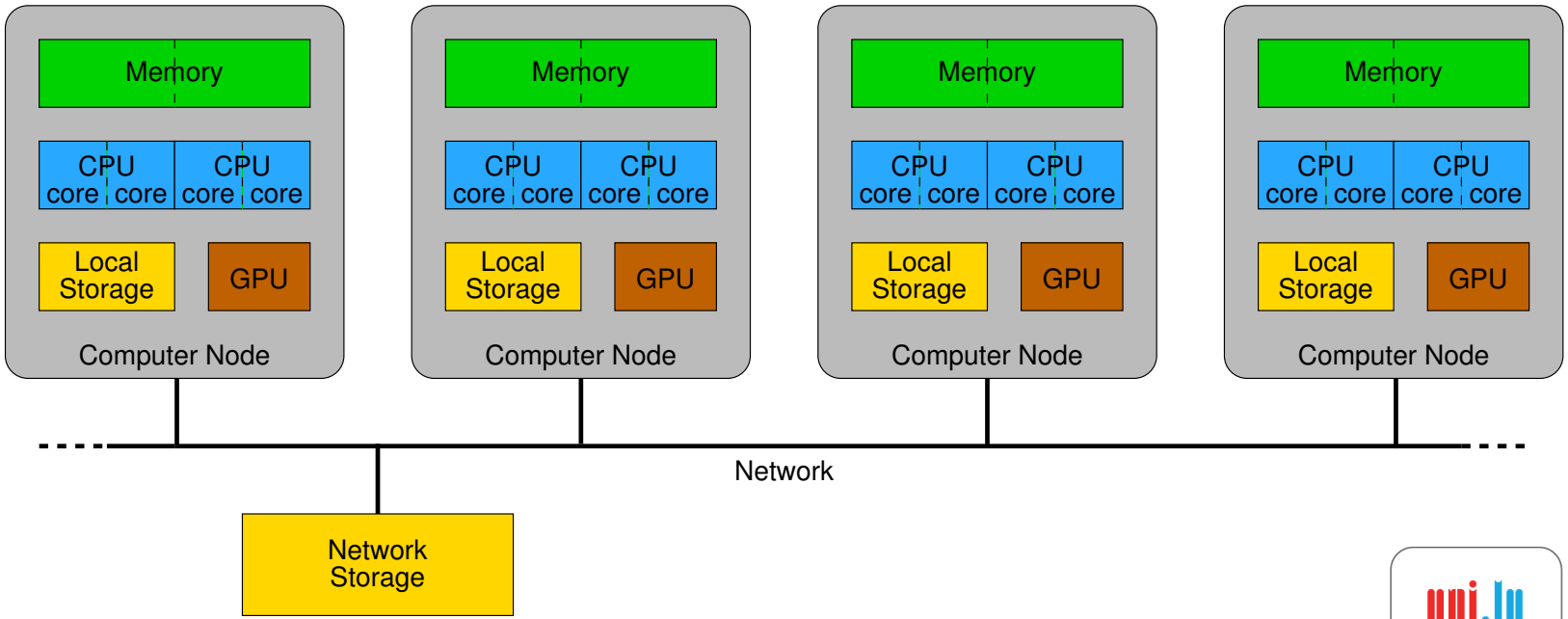
Outline

Getting faster: Identify performance bottlenecks

Note for code developers: The first bottleneck is your algorithm!

Know the hardware

- Computer nodes are connected using a fast interconnect
- Different types of resources:
  Processors, GPU, Memory, Storage, Network



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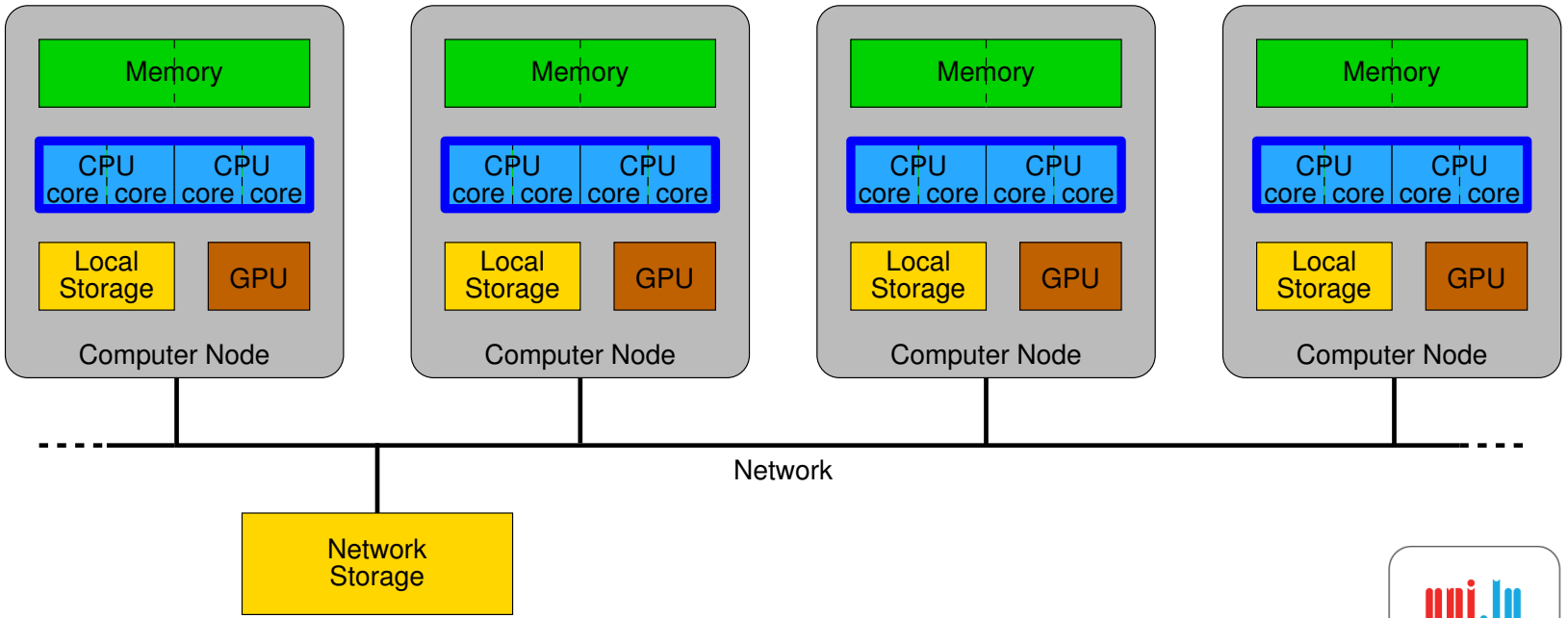

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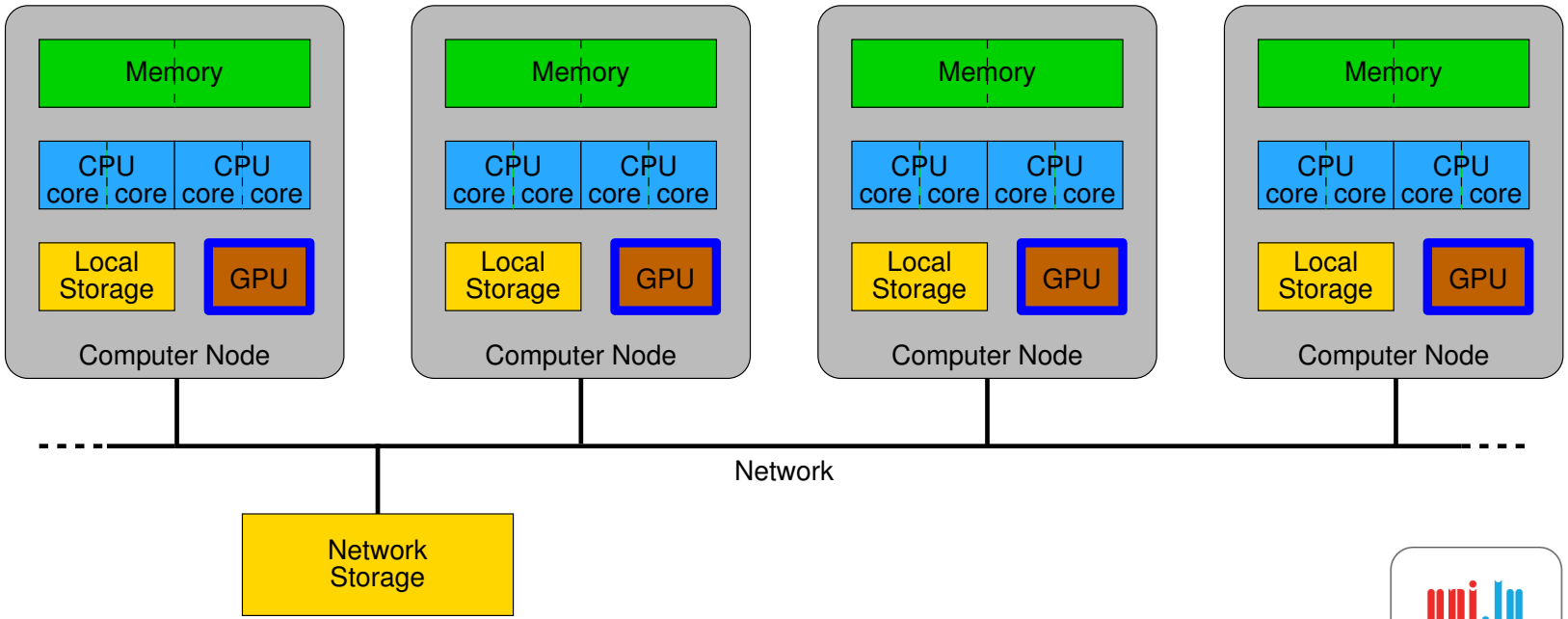

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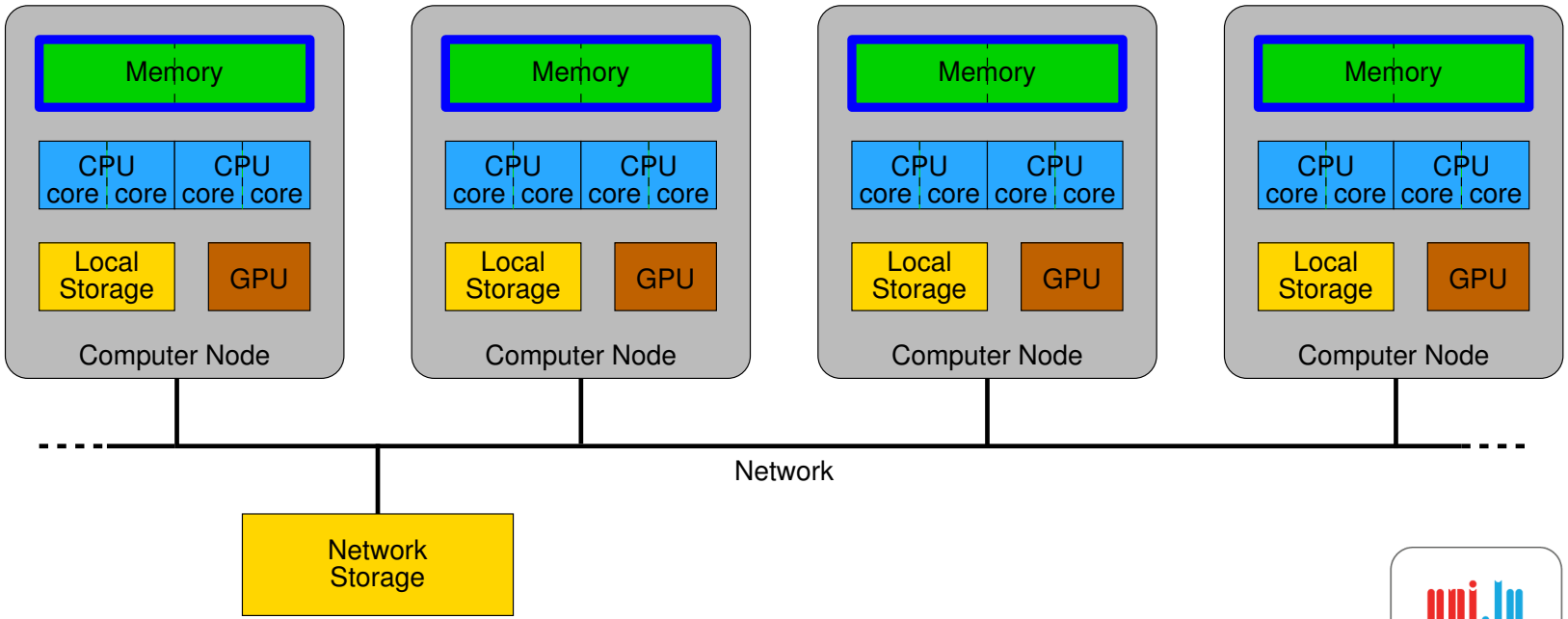

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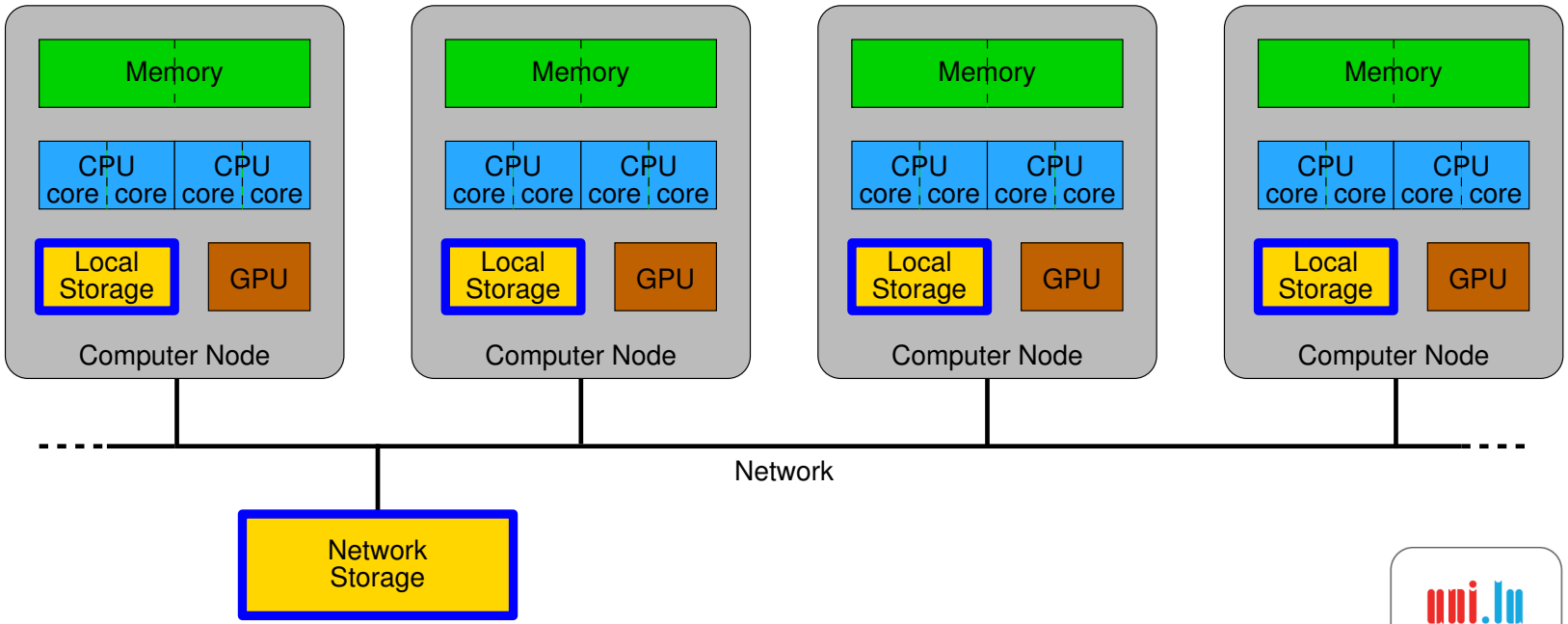

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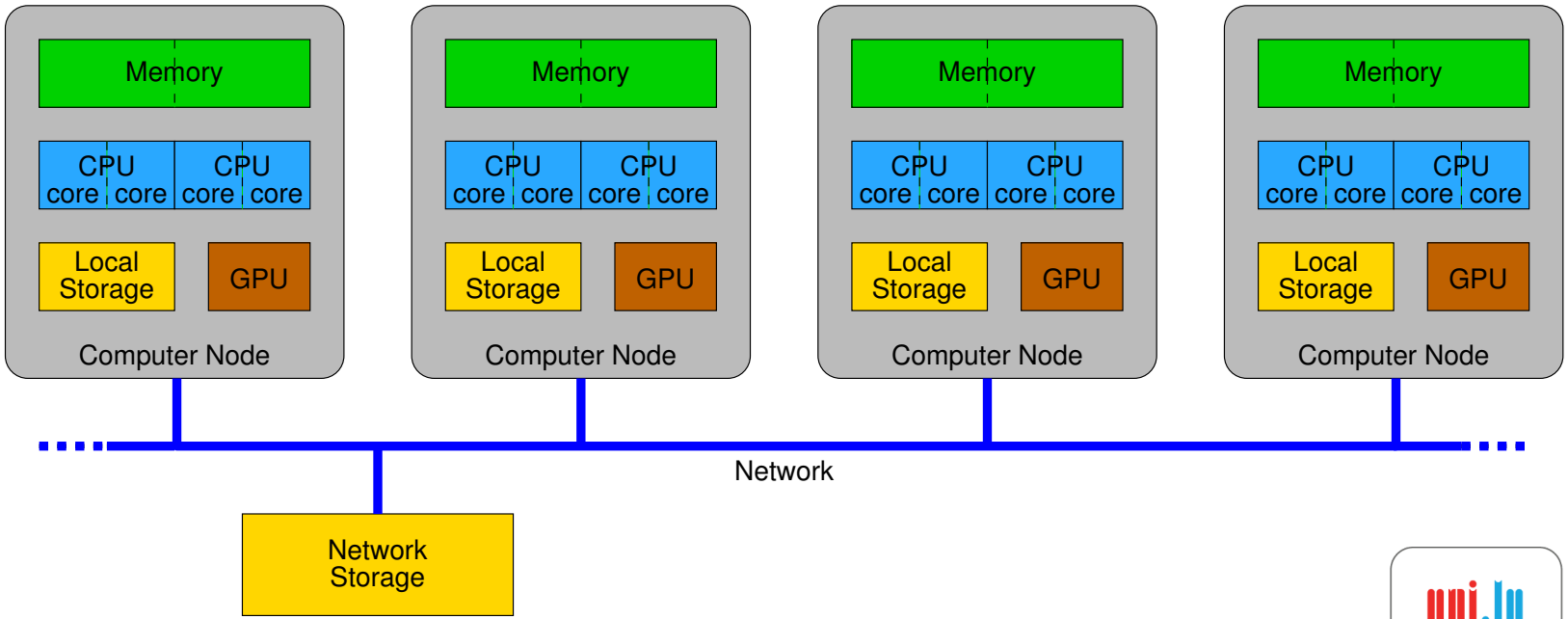
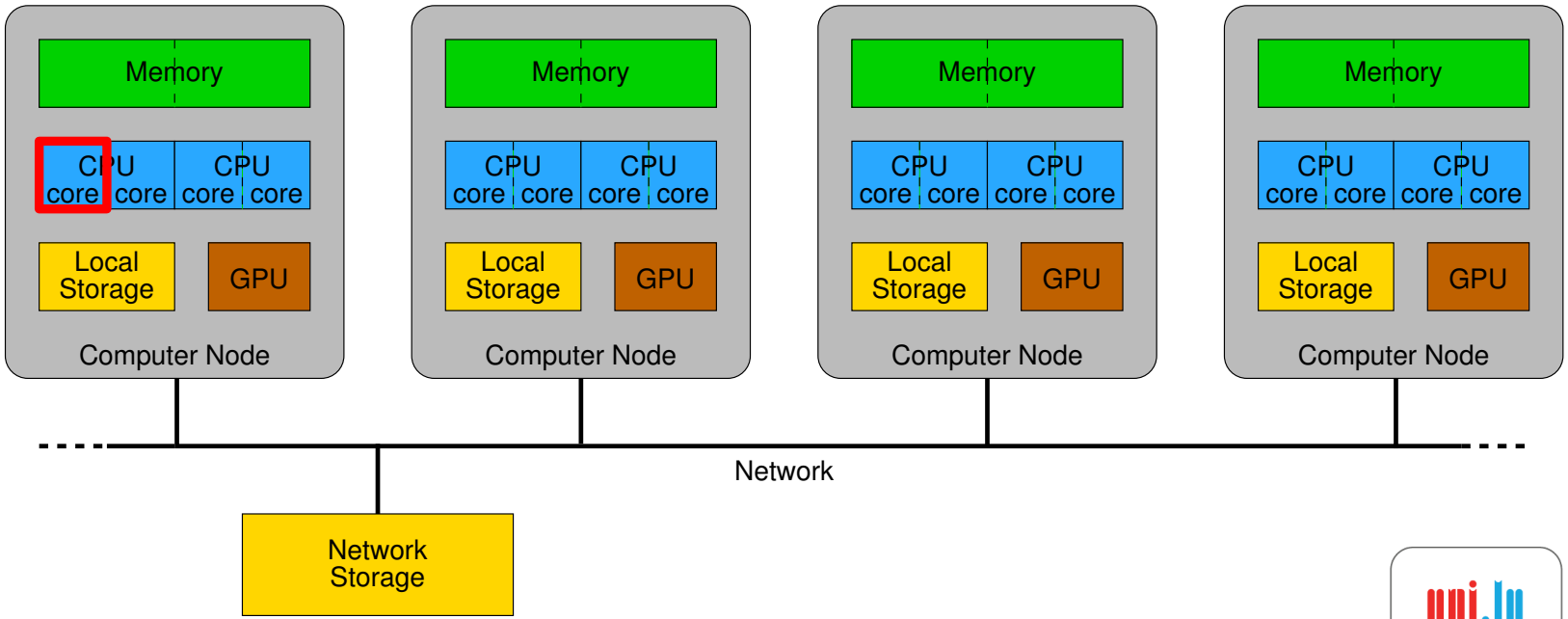


Processor bottleneck

Application is limited by the speed of the processor



Processor bottleneck

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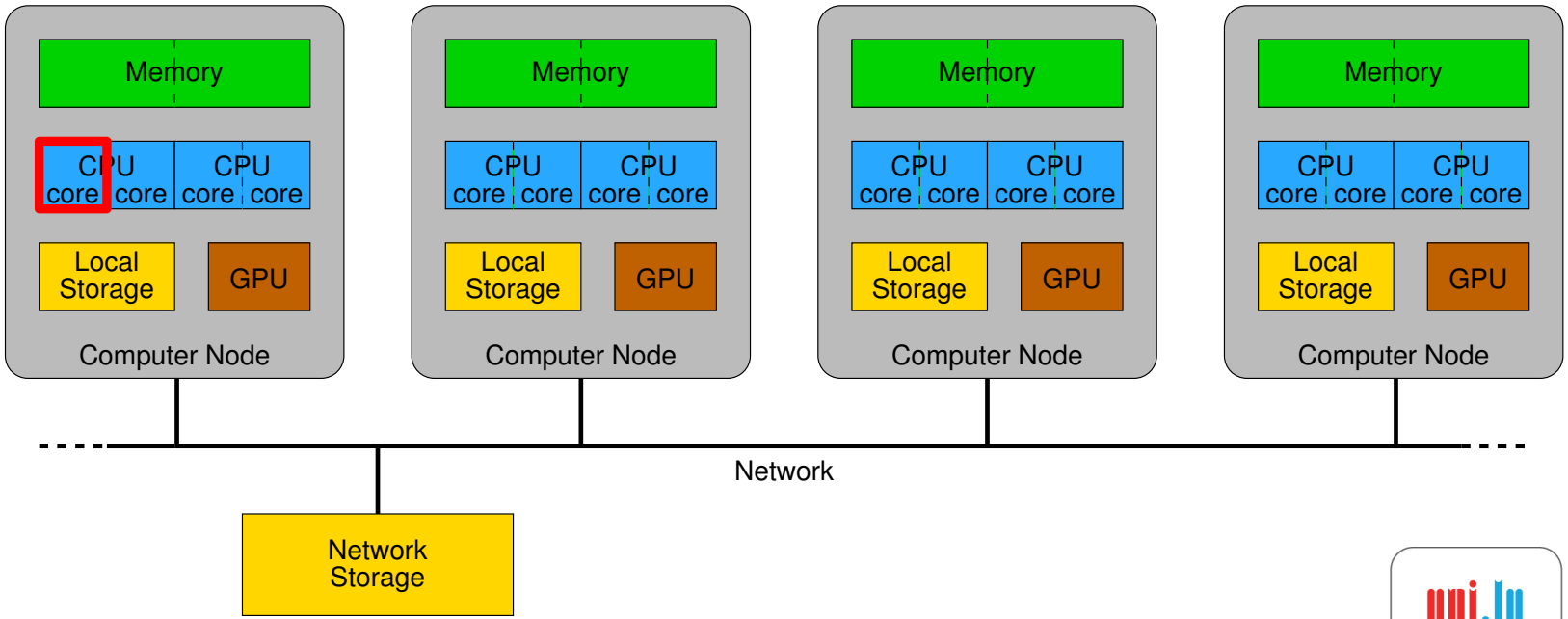
→ Optimize your code



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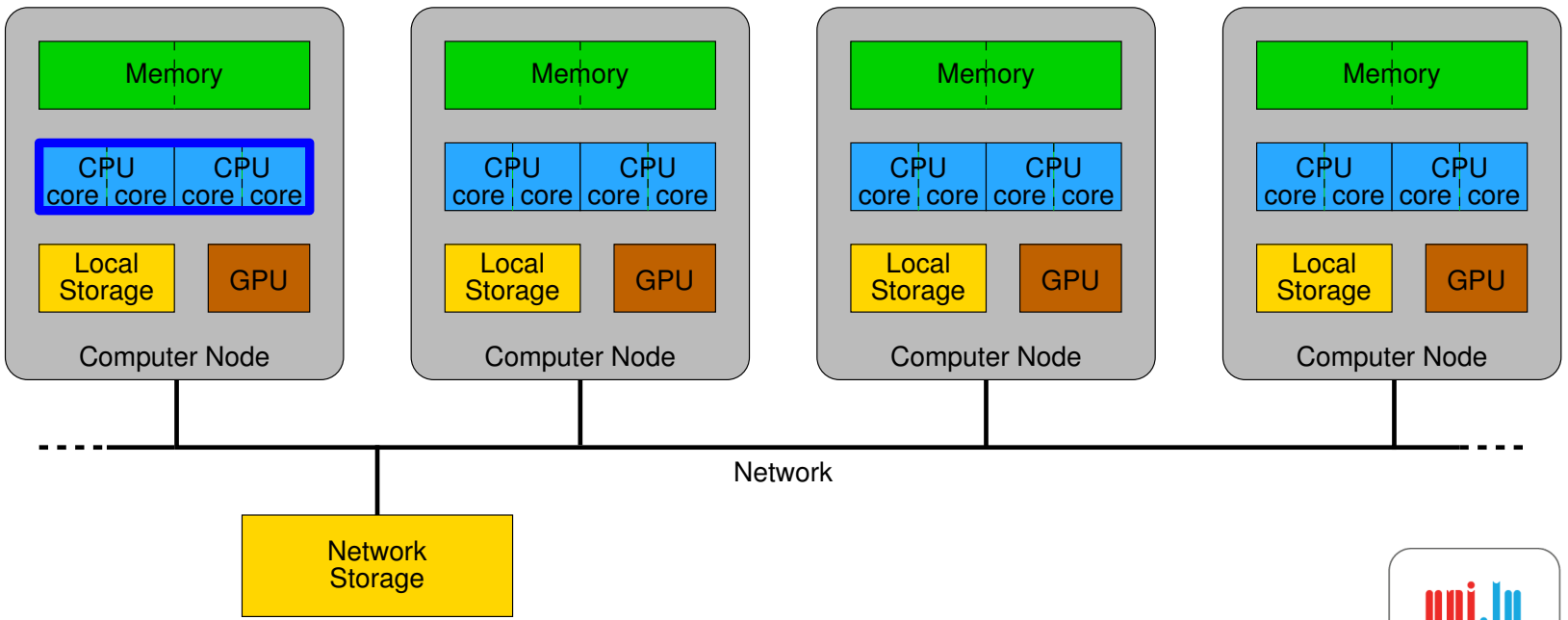
Application is limited by the speed of the processor

→ Optimize your code

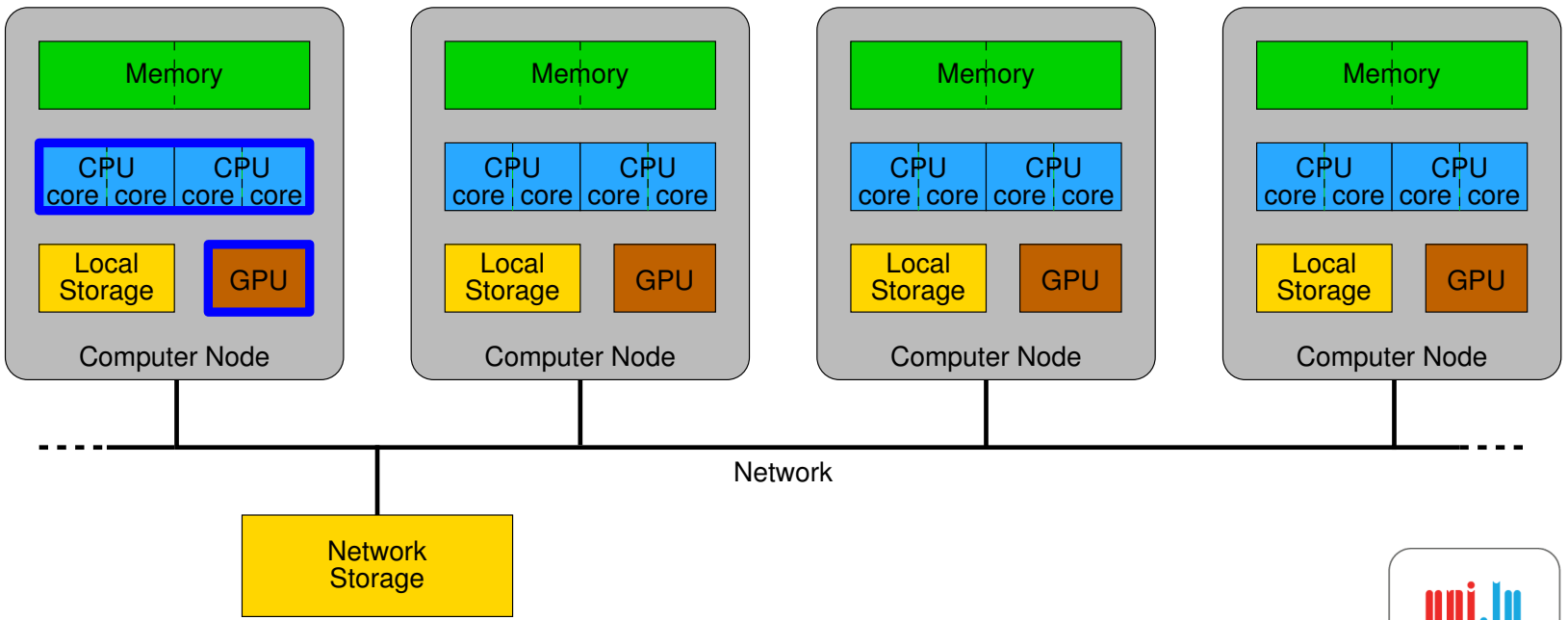
→ Parallel execution on a single node (pthread, OpenMP, Intel TBB)



Processor bottleneck

Application is limited by the speed of the processor

- → Optimize your code
- → Parallel execution on a single node (pthread, OpenMP, Intel TBB)
- → Use GPU accelerator (CUDA)



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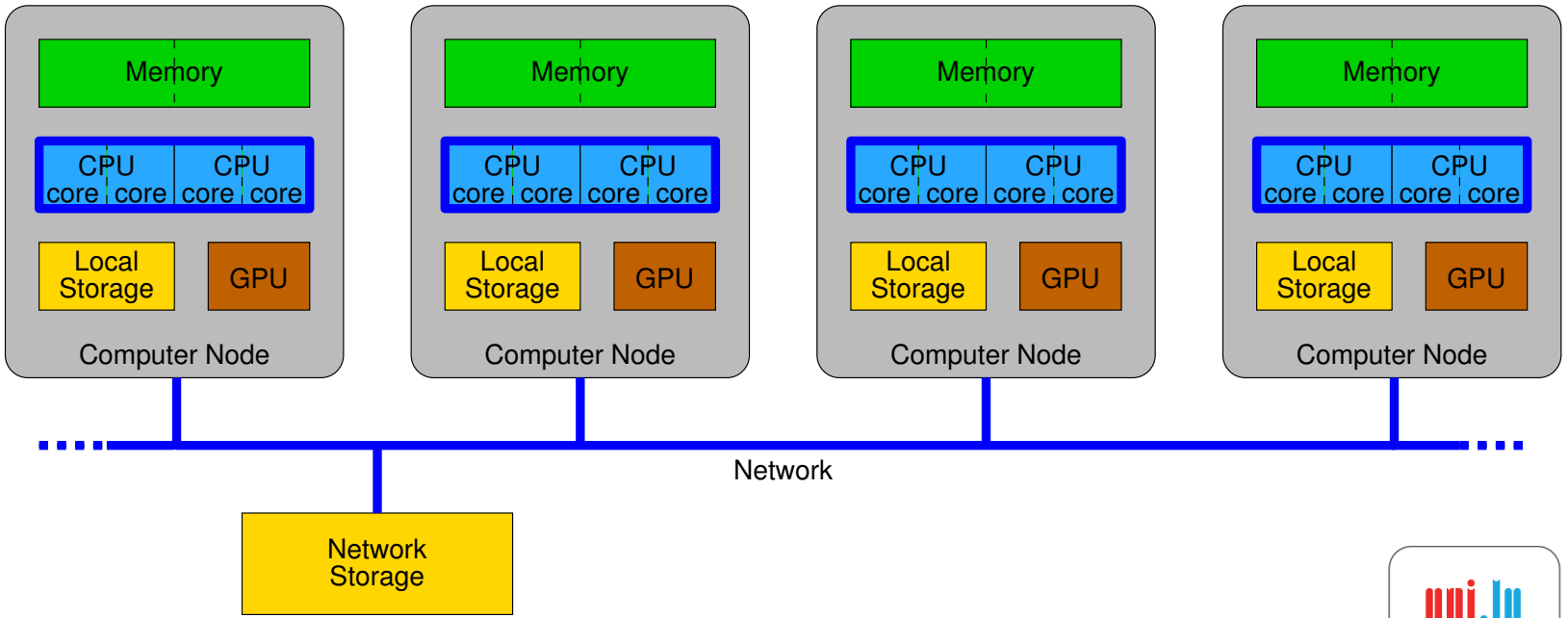
- → Parallel execution on multiple nodes (MPI)



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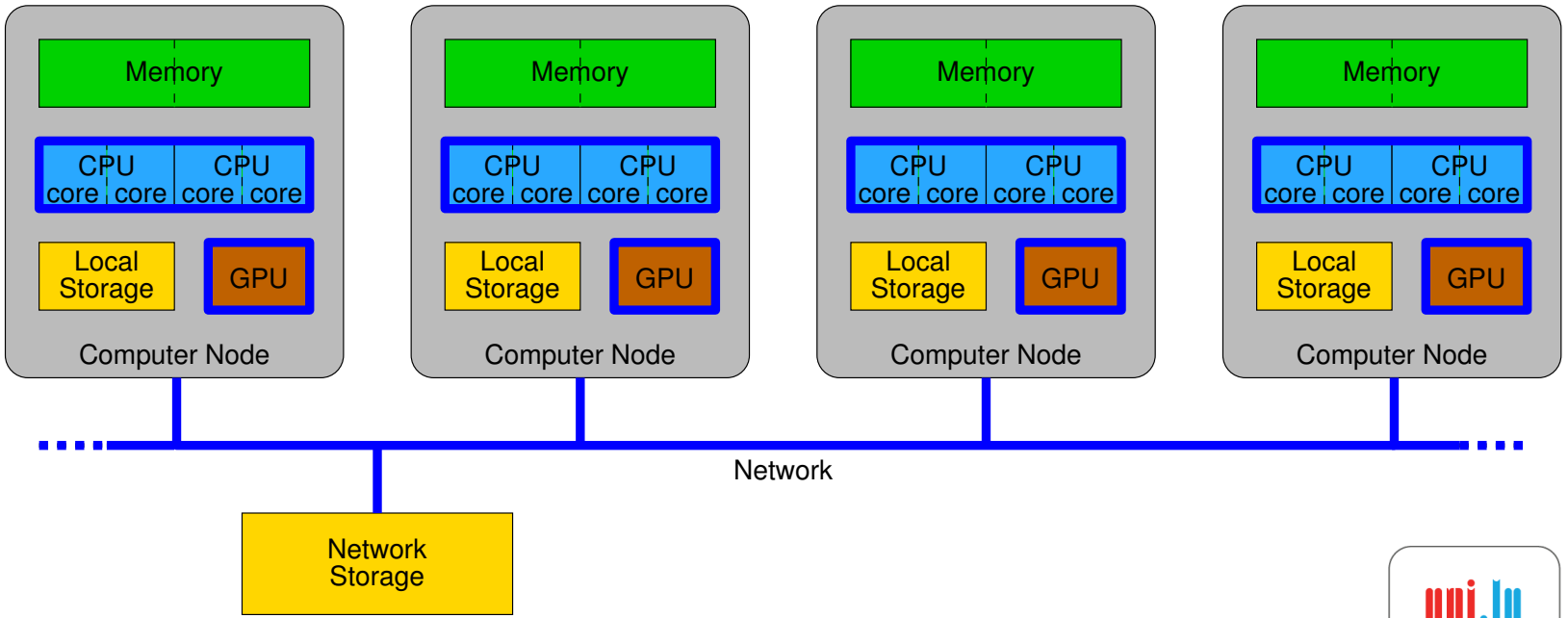
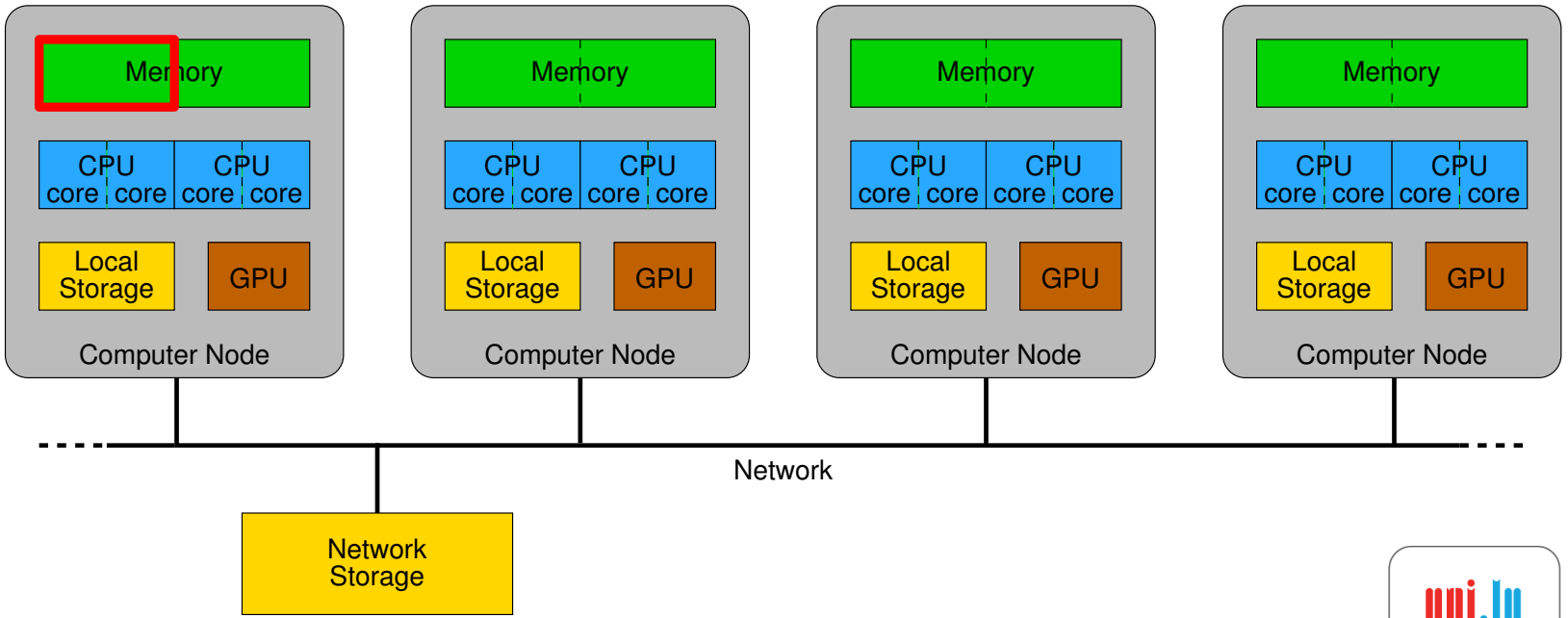
- → Parallel execution on a single node (pthread, OpenMP, Intel TBB)
- → Use GPU accelerator (CUDA)
- → Parallel execution on multiple nodes (MPI)
- → Parallel execution on multiple nodes with GPUs (MPI+CUDA)



Memory bottleneck

Application is limited by the size of the memory

- There is one memory bank per CPU

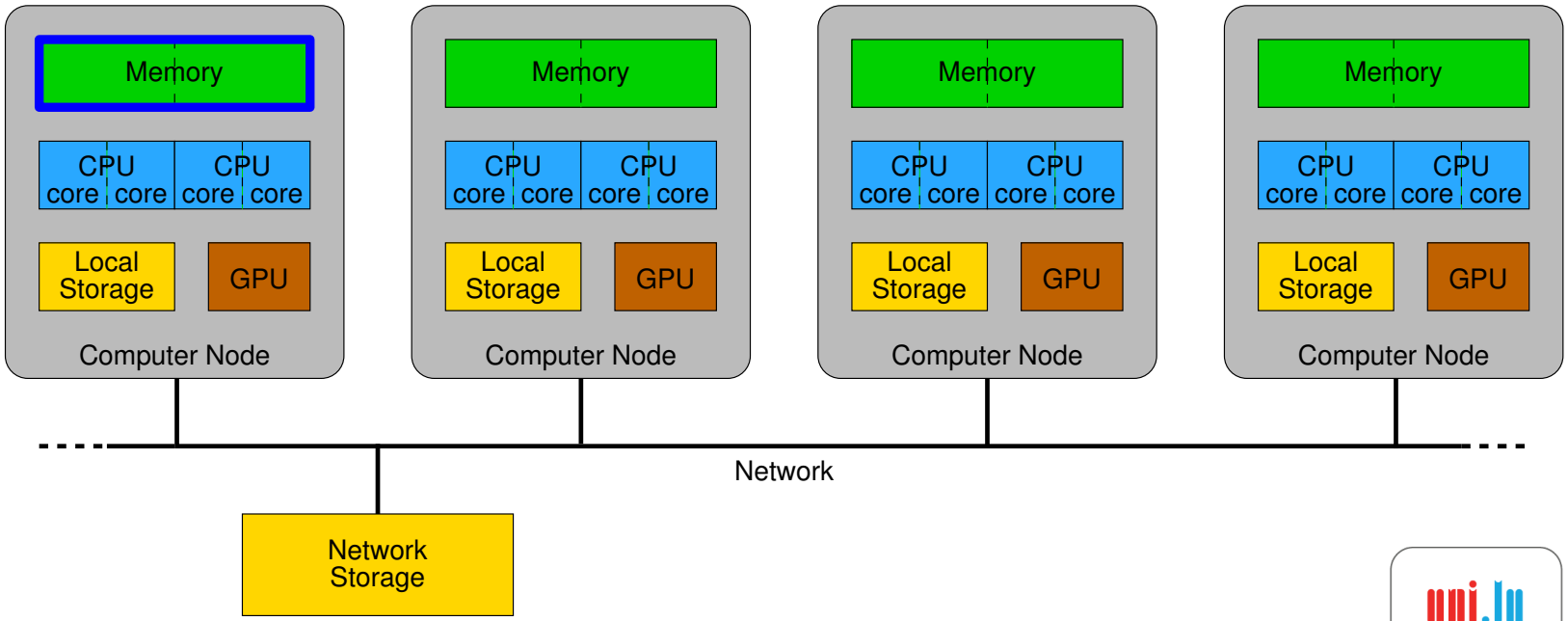


Memory bottleneck

Application is limited by the size of the memory

- There is one memory bank per CPU

→ Allocate all CPUs on a single node



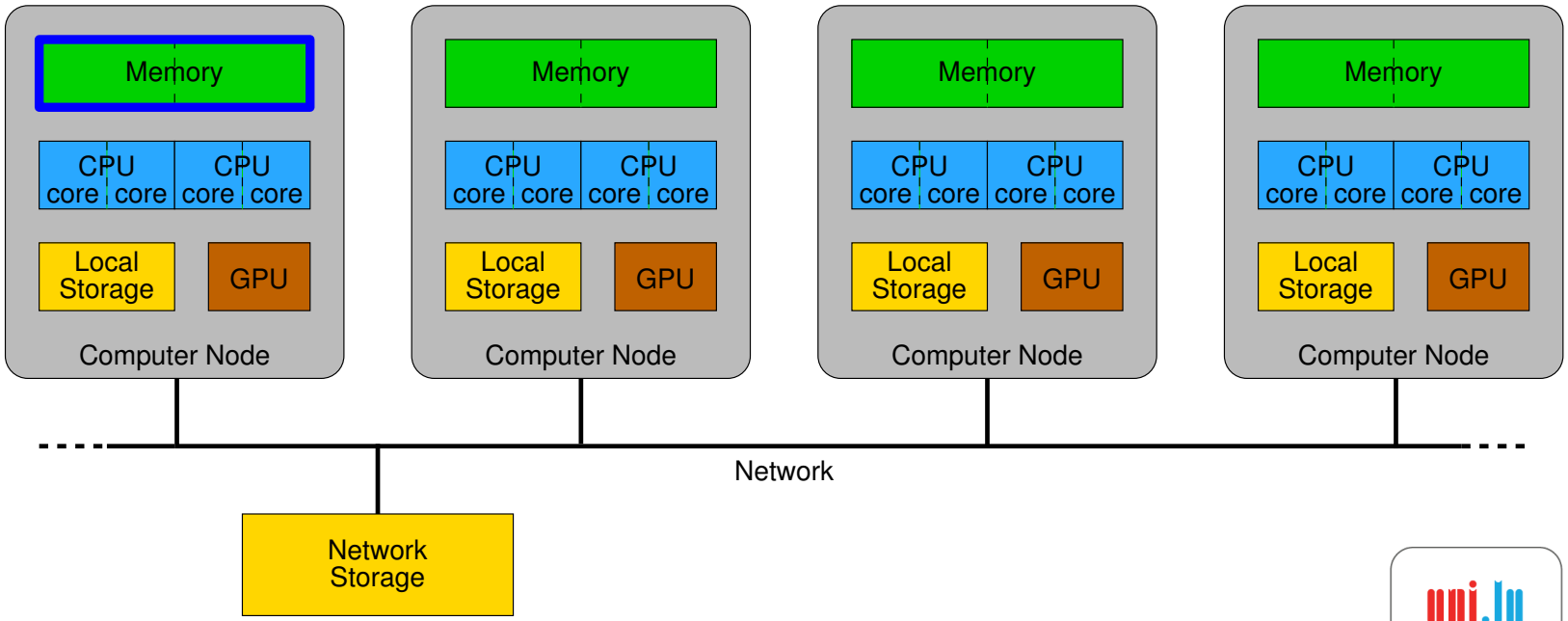
Memory bottleneck

Application is limited by the size of the memory

- There is one memory bank per CPU

→ Allocate all CPUs on a single node

→ Use a node with a bigger memory (4TB-memory node at UL)



Memory bottleneck

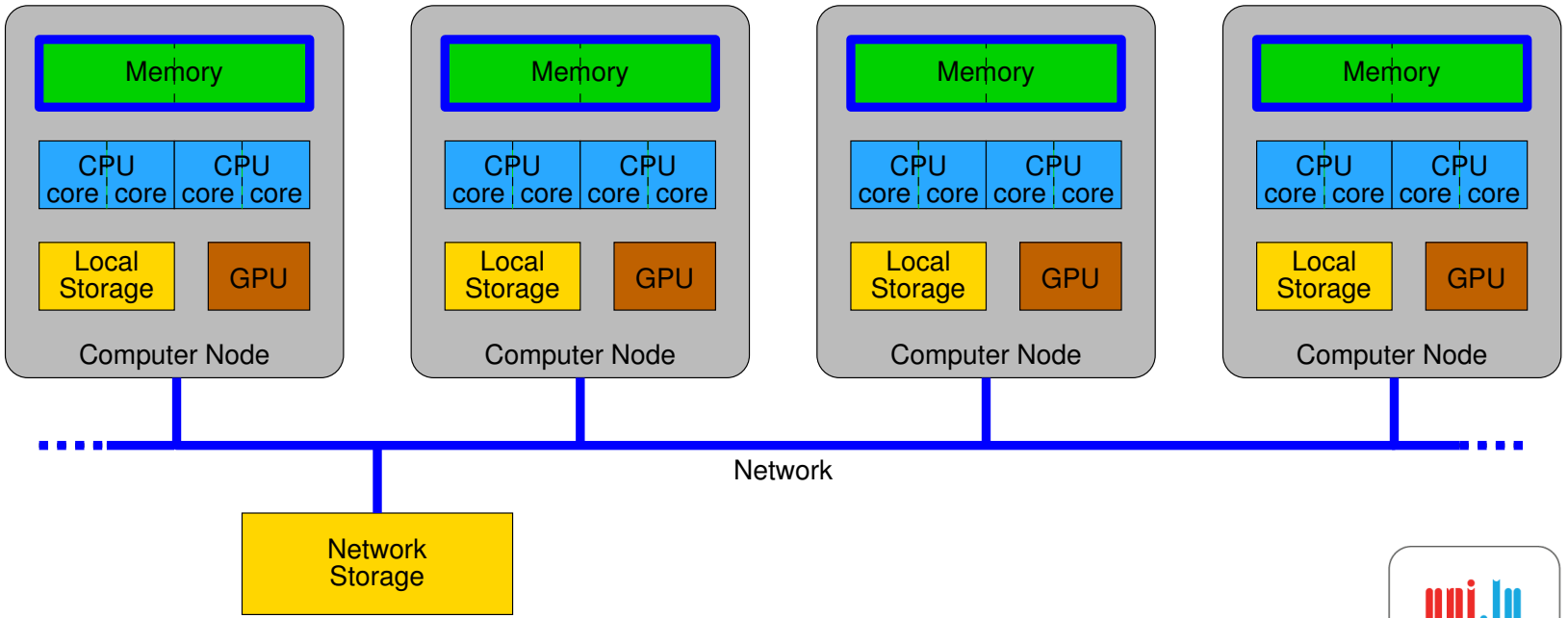
Application is limited by the size of the memory

- There is one memory bank per CPU

→ Allocate all CPUs on a single node

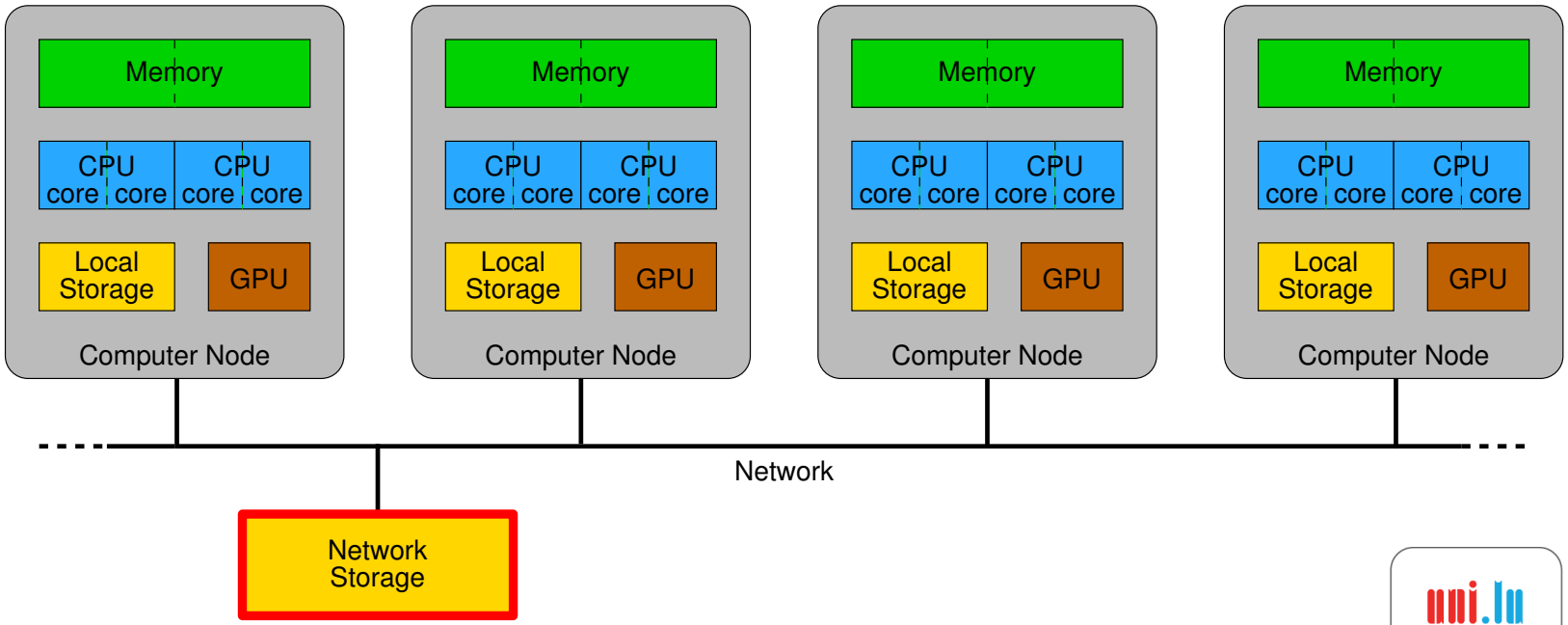
→ Use a node with a bigger memory (4TB-memory node at UL)

→ Distributed execution on multiple nodes (MPI)



Storage space bottleneck

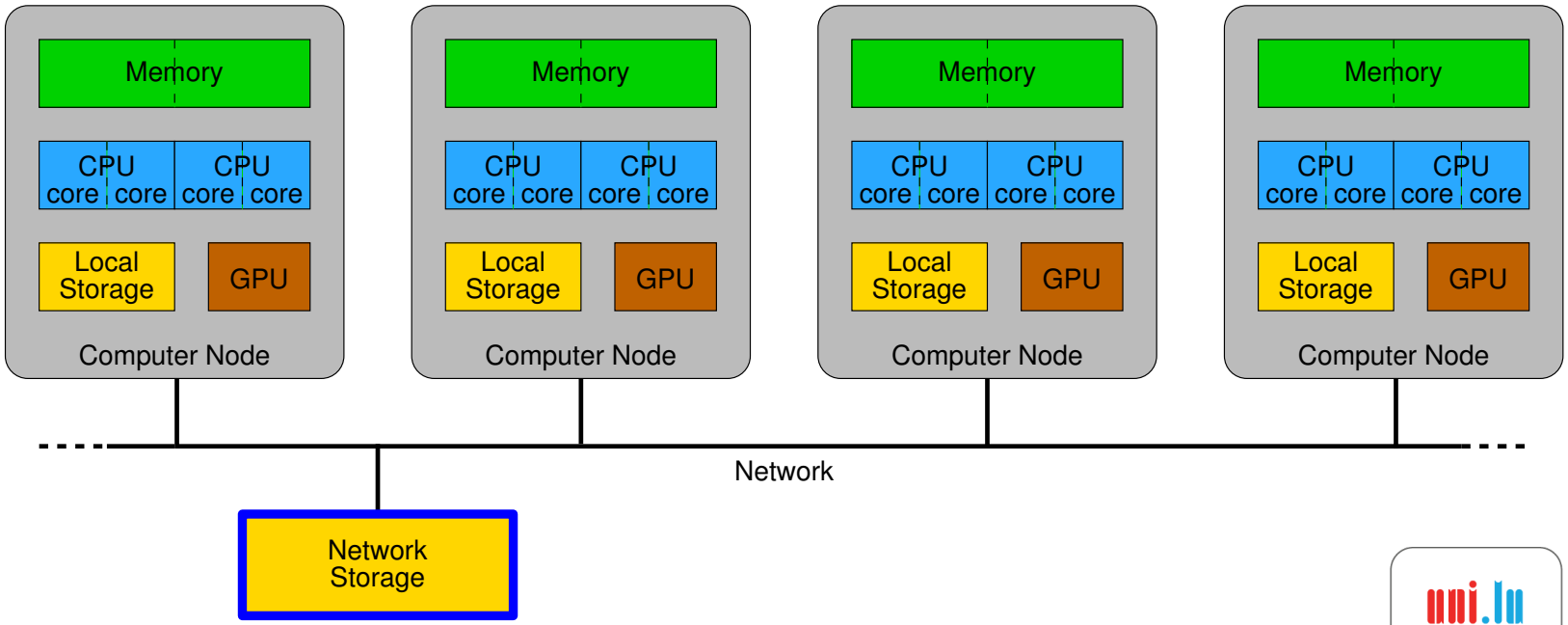
Application is limited by the available storage space



Storage space bottleneck

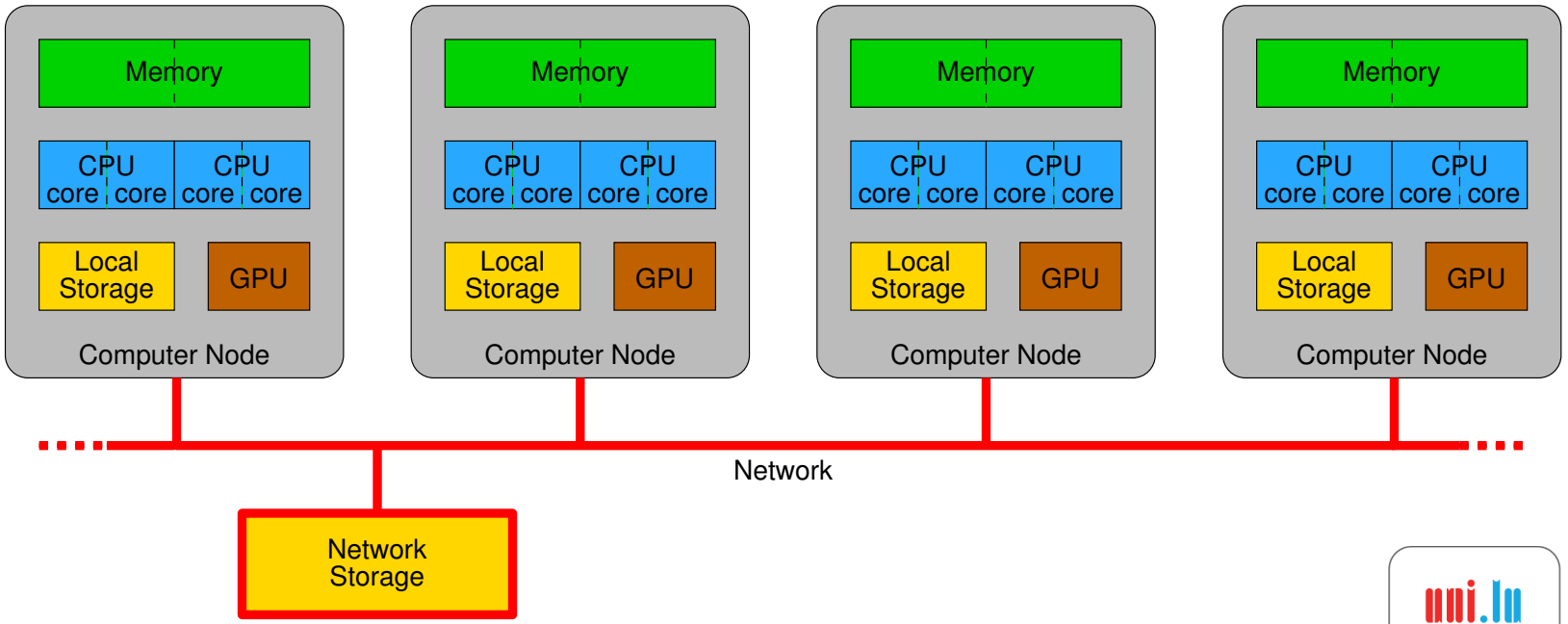
Application is limited by the available storage space

→ Use `$WORK` (3 TB) or `$SCRATCH` (10 TB)
(no backup!)



Storage speed bottleneck

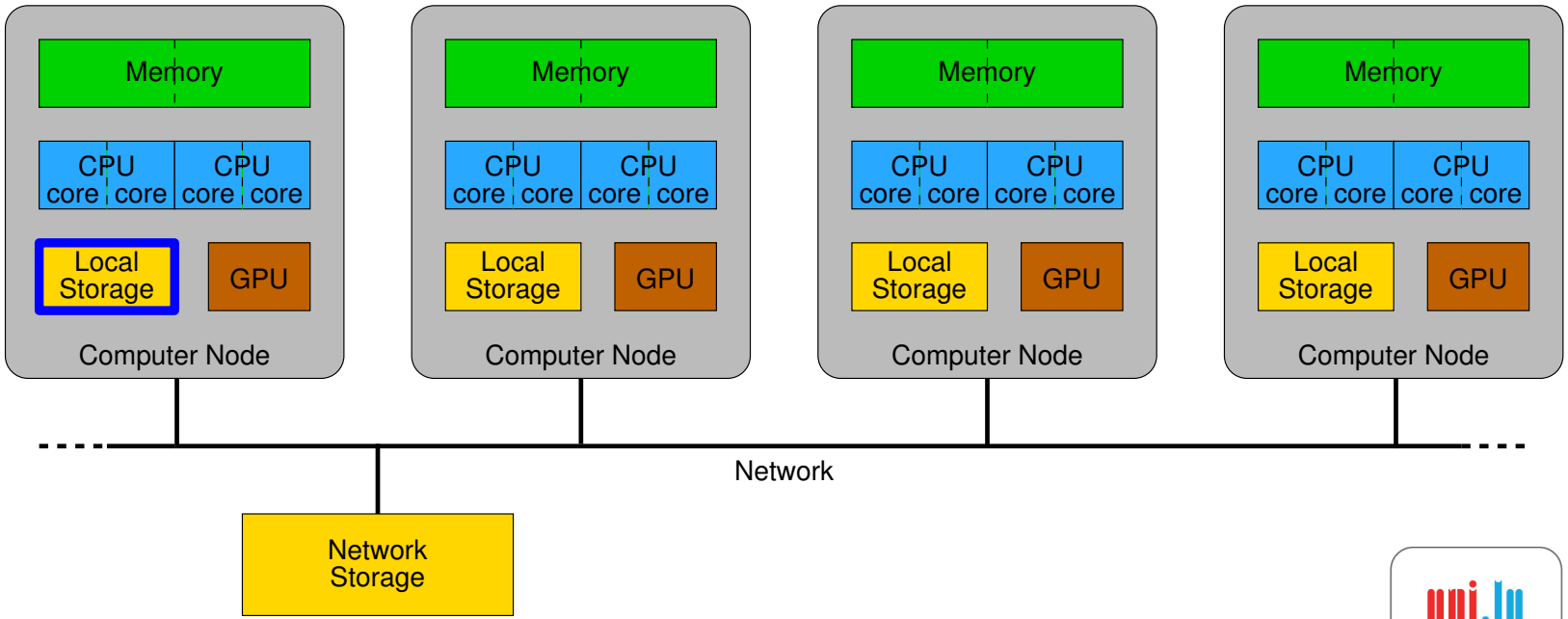
Application is limited by the speed of the storage



Storage speed bottleneck

Application is limited by the speed of the storage

→ Use local storage instead of network storage
(copy data back to network storage after execution)

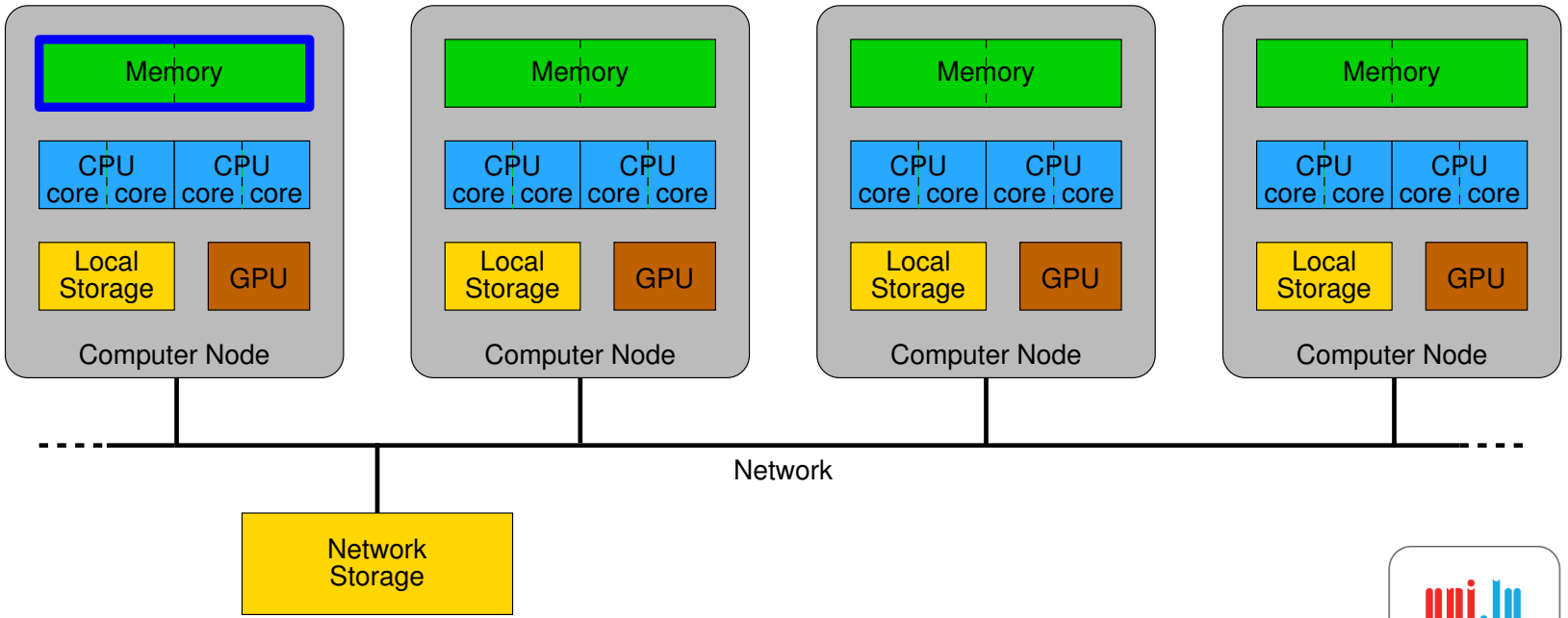


Storage speed bottleneck

Application is limited by the speed of the storage

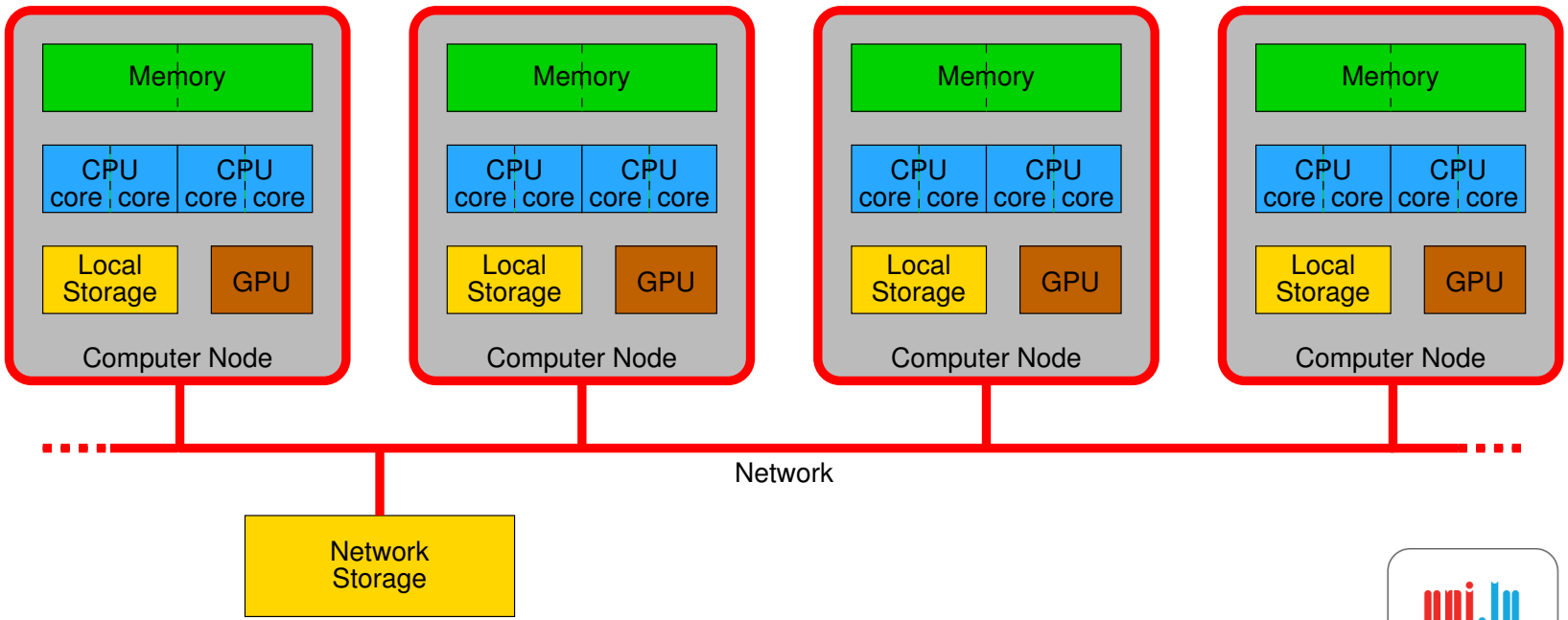
→ Use local storage instead of network storage
(copy data back to network storage after execution)

→ Use local memory, *eg* `/dev/shm` (space is limited!)



Network bottleneck

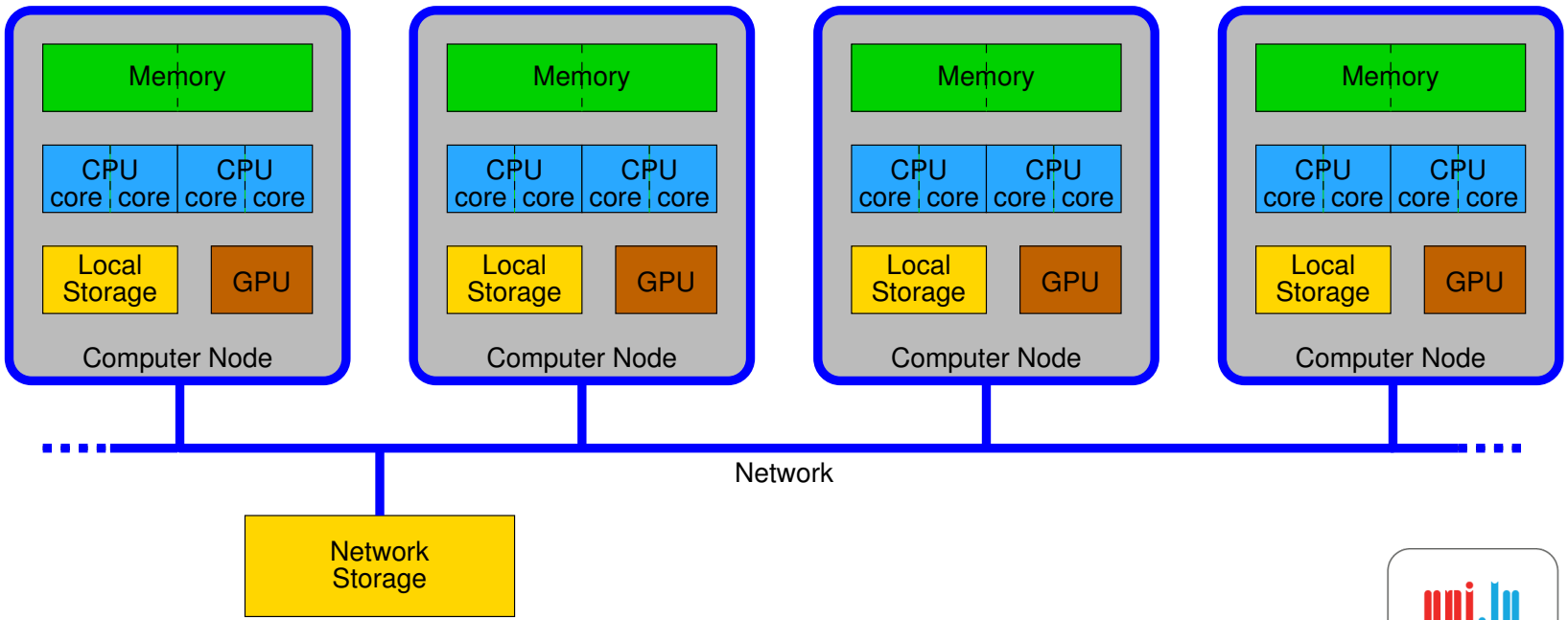
Application is limited by the speed of the network
(too many communications)



Network bottleneck

Application is limited by the speed of the network (too many communications)

→ Use Infiniband network instead of Ethernet

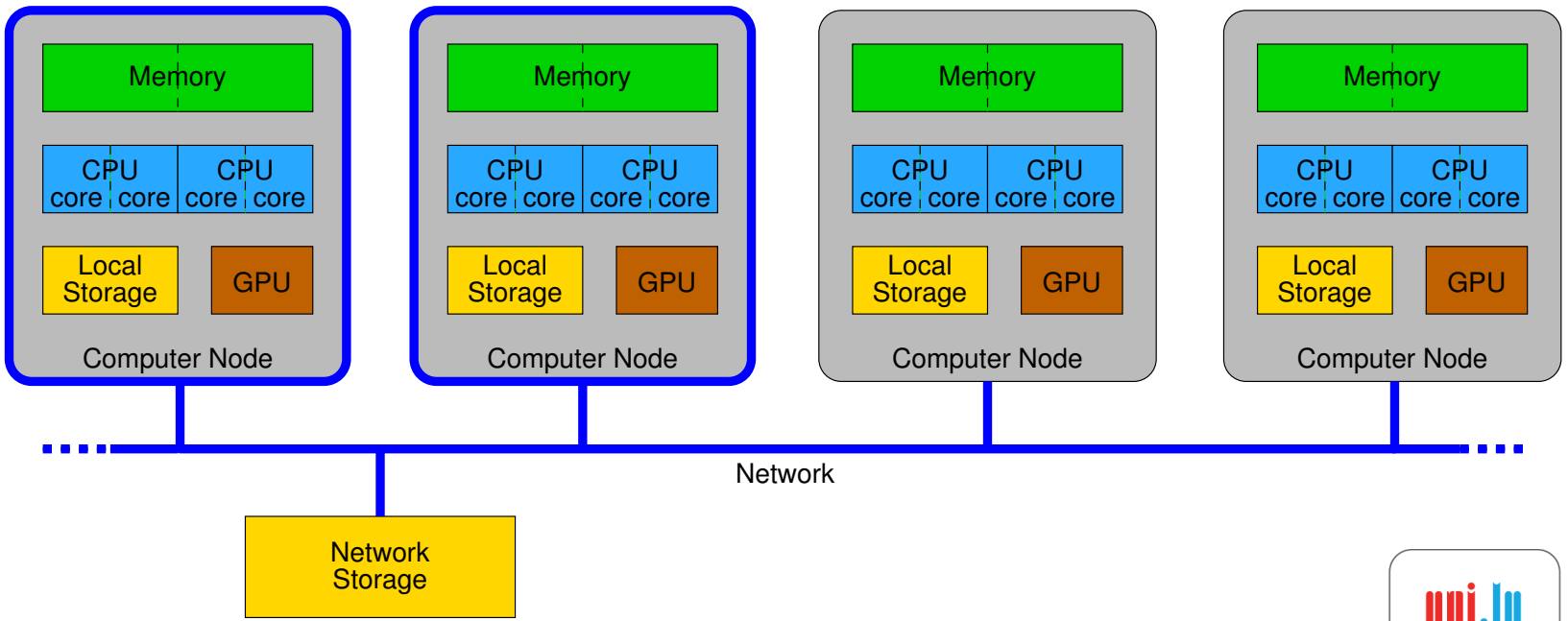


Network bottleneck

Application is limited by the speed of the network (too many communications)

→ Use Infiniband network instead of Ethernet

→ Reduce the number of nodes



Quick Tips for classic use-cases

Sequential job — PS 2A, PS 5C

→ Parallelization: OpenMP, MPI

→ Use accelerators: CUDA

Long job — PS 6C

→ Checkpoint/Restart: BLCR

Large number of jobs — PS 6C

eg parametric studies

→ Parallel launcher

→ Best effort queue

→ OAR Job containers

Visualization / Rendering

→ GPU nodes with graphic session using XCS portal

Keynote 4, PS 6B

MATLAB — PS 2B, PS 3B

→ Parallelization: Parallel Computing Toolbox

→ Checkpoint/Restart: `save()`/`load()` functions

R — PS 3C

→ Use optimized data structure / package: `data.table` / `plyr`

→ Parallelization: packages parallel, Rmpi, snow

Python

→ Library for scientific computing: NumPy, Scipy, matplotlib

→ Parallelization: multiprocessing library

→ Use latest version of Python

...