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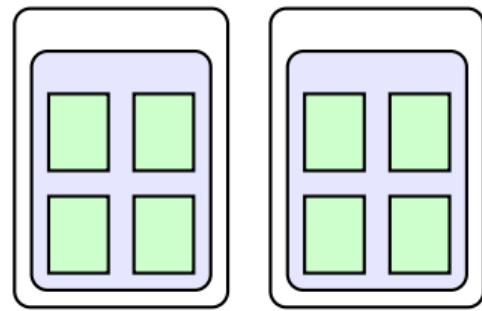
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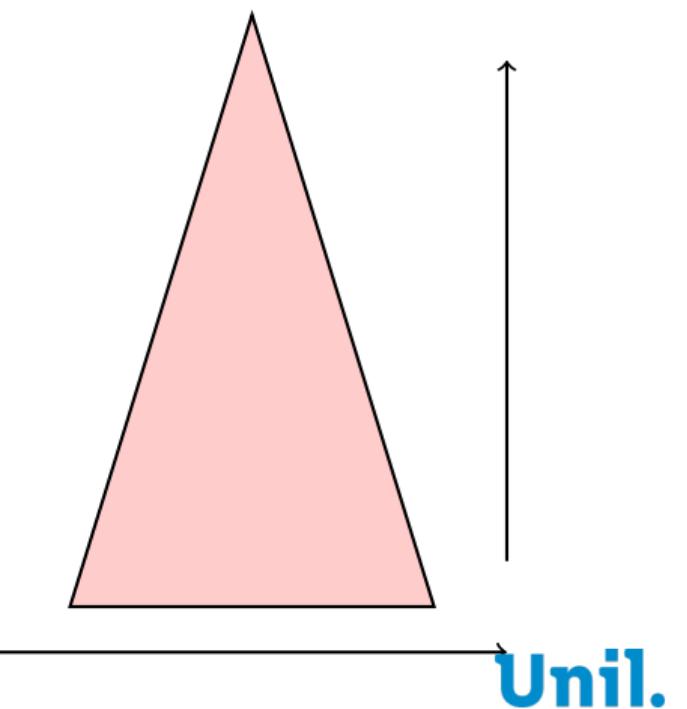


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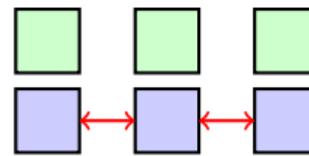
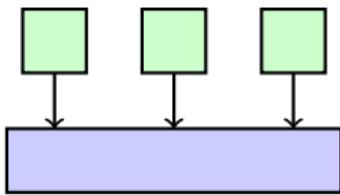
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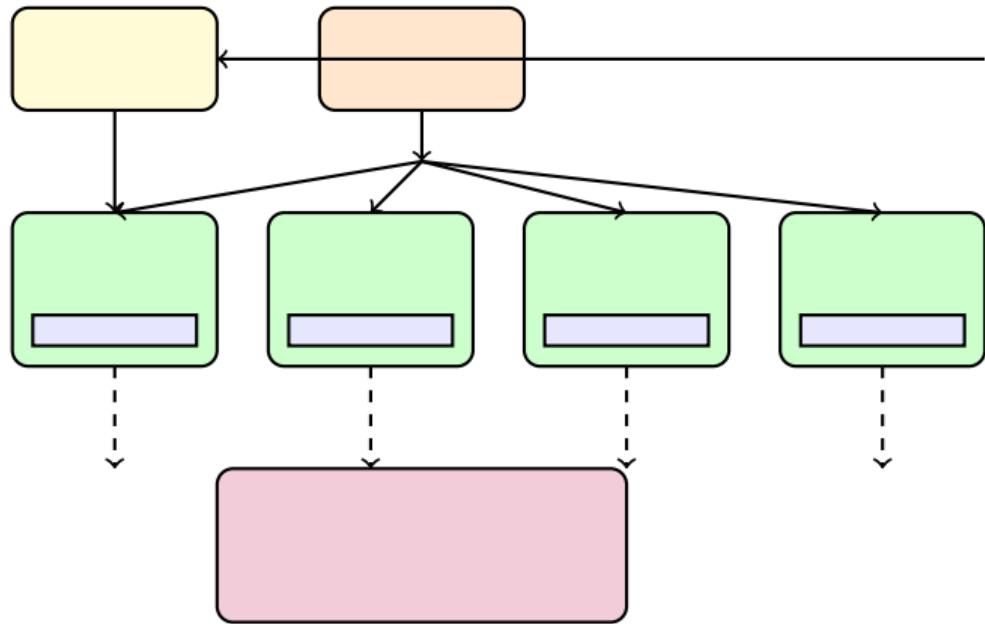
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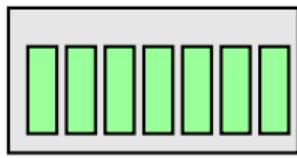
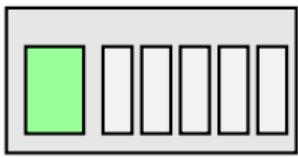
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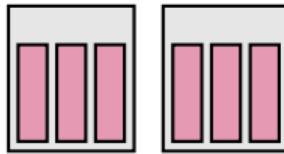
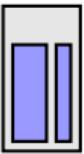
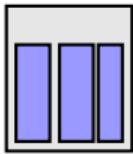




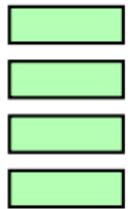
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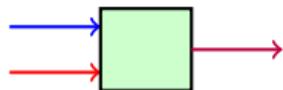
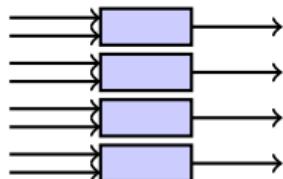


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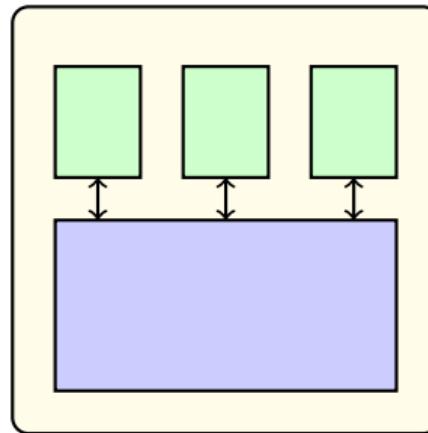
$$C[0 : 3] = A[0 : 3] + B[0 : 3]$$



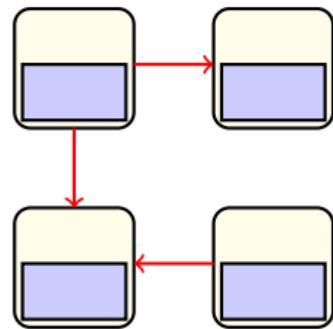
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```
#pragma omp parallel for
for (int i = 0; i < N; i++) {
    c[i] = a[i] + b[i];
}
```

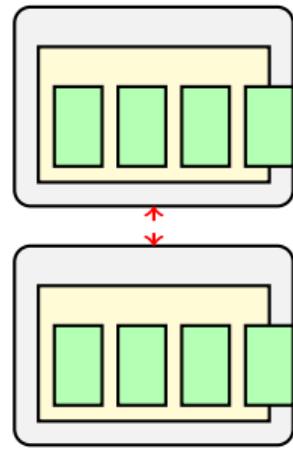


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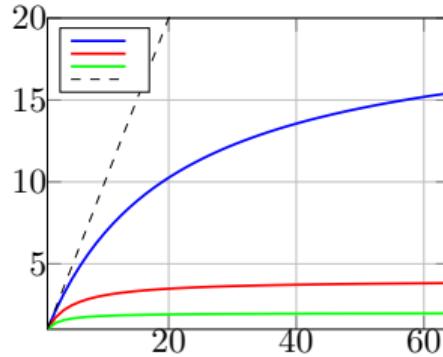
- ▶ MPI_Send
- ▶ MPI_Recv
- ▶ MPI_Bcast
- ▶ MPI_Reduce

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



- ▶ $S(n)n$
- ▶ p
- ▶ $(1-p)$

- ▶
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```
sbatch script.sh
squeue
squeue -u $USER
scancel <jobid>
sinfo
srun command
scontrol show job <jobid>
sacct
salloc

▶ -l
▶ --start
▶ -t RUNNING
```

```
#!/bin/bash
#SBATCH --job-name=myjob
#SBATCH --output=output_%j.txt
#SBATCH --error=error_%j.txt
#SBATCH --time=01:00:00
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=4
#SBATCH --mem=8G

# Load modules
module load python/3.9

# Set environment
export OMP_NUM_THREADS=4

# Run application
python my_script.py
```

- ▶ --job-name
- ▶ --output/--error
- ▶ --time
- ▶ --nodes
- ▶ --ntasks
- ▶ --cpus-per-task
- ▶ --mem
- ▶ --mem-per-cpu
- ▶ %j

```
#!/bin/bash

#SBATCH --job-name=serial_job
#SBATCH --output=serial_%j.log
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --mem=2G
#SBATCH --time=00:30:00

echo "Running on host: $(hostname)"
echo "Job ID: $SLURM_JOB_ID"
echo "Number of cores: $SLURM_CPUS_PER_TASK"

python my_serial_script.py
```

```
#!/bin/bash

#SBATCH --job-name=openmp_job
#SBATCH --output=openmp_%j.log
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=16
#SBATCH --mem=32G
#SBATCH --time=02:00:00

module load gcc/11.2.0

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
echo "Using $OMP_NUM_THREADS OpenMP threads"
```

```
#!/bin/bash

#SBATCH --job-name=mpi_job
#SBATCH --output=mpi_%j.log
#SBATCH --nodes=4
#SBATCH --ntasks=64
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=2G
#SBATCH --time=04:00:00

module load openmpi/4.1.1

echo "Running on $SLURM_NNODES nodes"
echo "Total tasks: $SLURM_NTASKS"
```

```
#!/bin/bash

#SBATCH --job-name=hybrid_job
#SBATCH --output=hybrid_%j.log
#SBATCH --nodes=4
#SBATCH --ntasks=16
#SBATCH --cpus-per-task=8
#SBATCH --mem=256G
#SBATCH --time=06:00:00

module load gcc/11.2.0 openmpi/4.1.1

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
echo "MPI tasks: $SLURM_NTASKS"
```



```
#!/bin/bash
#SBATCH --job-name=array_job
#SBATCH --output=job_%A_%a.log
#SBATCH --array=1-100
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=1
#SBATCH --mem=2G
#SBATCH --time=01:00:00

# SLURM_ARRAY_TASK_ID contains
# the current array index (1-100)
PARAM=$SLURM_ARRAY_TASK_ID

echo "Processing parameter: $PARAM"
python process.py --id $PARAM
```

► %A

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```
# Interactive single command
srun --ntasks=1 \
    --cpus-per-task=4 \
    --mem=8G \
    --time=01:00:00 \
    python my_script.py
```



```
# Allocate resources
salloc --nodes=1 \
    --ntasks=4 \
    --mem=16G \
    --time=02:00:00

# Now on compute node
hostname
module load python
python
# ... work interactively ...
exit # Release resources
```



```
threadingmultiprocessingjoblib  
mpi4py  
numpynumba  
Threads.@threads@spawn  
MPI.jl  
Distributed.jl@distributed  
parallelforeach  
RmpipbdMPI
```

```
from concurrent.futures import ThreadPoolExecutor
import numpy as np

def compute(x):
    # Good for I/O-bound tasks
    return np.sqrt(x)

with ThreadPoolExecutor(max_workers=4) as executor:
    results = executor.map(compute, range(100))
```

```
from multiprocessing import Pool

def compute(x):
    # Good for CPU-bound tasks
    return x ** 2

with Pool(processes=4) as pool:
    results = pool.map(compute, range(100))
```



```
# For multiprocessing
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=4

# Set in Python
from multiprocessing import cpu_count
import os
n_cores = int(os.getenv(
    'SLURM_CPUS_PER_TASK',
    cpu_count()))
```

```
from mpi4py import MPI
import numpy as np

comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

# Each process computes part
n_local = 1000
data = np.random.rand(n_local)
local_sum = np.sum(data)

# Reduce to get total sum
total_sum = comm.reduce(local_sum,
                        op=MPI.SUM,
                        root=0)

if rank == 0:
    print(f"Total: {total_sum}")
```

```
#!/bin/bash
#SBATCH --ntasks=16
#SBATCH --cpus-per-task=1
#SBATCH --mem-per-cpu=2G
#SBATCH --time=01:00:00

module load openmpi python/3.9

mpirun python my_mpi_script.py
```

► mpirun

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```
using Base.Threads

# Set threads with environment variable
# export JULIA_NUM_THREADS=4

function parallel_sum(arr)
    result = zeros(nthreads())
    @threads for i in eachindex(arr)
        tid = threadid()
        result[tid] += arr[i]
    end
    return sum(result)
end
```

```
using Distributed

addprocs(4) # Add 4 workers

@everywhere function compute(x)
```

```
#!/bin/bash
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=8
#SBATCH --mem=16G
#SBATCH --time=02:00:00

module load julia/1.8

# For threading
export JULIA_NUM_THREADS=$SLURM_CPUS_PER_TASK

julia my_script.jl
```

```
using MPI

MPI.Init()
comm = MPI.COMM_WORLD
rank = MPI.Comm_rank(comm)
size = MPI.Comm_size(comm)
```

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```
library(foreach)
library(doParallel)

# Register parallel backend
cl <- makeCluster(4)
registerDoParallel(cl)

# Parallel loop
results <- foreach(i=1:100, .combine=c) %dopar% {
  # Computation
  i^2
}

stopCluster(cl)
```

```
library(parallel)

# Detect cores
ncores <- detectCores()
```

```
#!/bin/bash
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=8
#SBATCH --mem=16G
#SBATCH --time=01:00:00

module load r/4.2

# Set cores from SLURM
export R_NCORES=$SLURM_CPUS_PER_TASK

Rscript my_script.R
```

```
# Get cores from environment
ncores <- as.integer(Sys.getenv("R_NCORES", "1"))

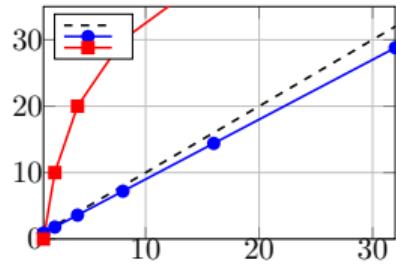
cl <- makeCluster(ncores)
# ... rest of code
```

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► >



`sbatch`

`squeue`

- ▶ $\sum_{i=1}^N i^2$
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```
sinfo  
sacct--mem  
--time  
module availmodule load
```

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- ▶ sallocsrun
- ▶

- ▶ /usr/bin/time -v



- ▶ = × × 1.3



- ▶ $T \approx \frac{T}{N \times}$



► %j

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- ▶ <https://slurm.schedmd.com/>
- ▶
- ▶ man sbatchman srun

- ▶ <https://www.hpc-carpentry.org/>
- ▶ <https://www.xsede.org/for-users/training>
- ▶ <https://www.openmp.org/resources/tutorials-articles/>
- ▶ <https://mpitutorial.com/>

- ▶ gprofperfIntel VTune
- ▶ gdbvalgrindDDT
- ▶ squeueqesacctcontrol

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