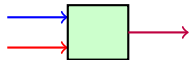
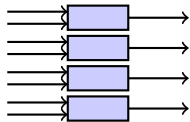
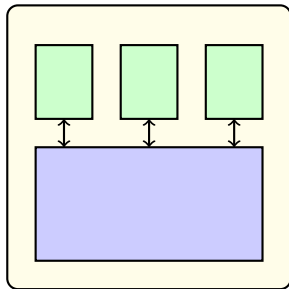


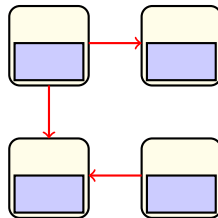


$$C[0 : 3] = A[0 : 3] + B[0 : 3]$$

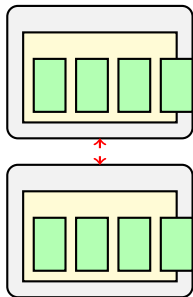




```
#pragma omp parallel for
for (int i = 0; i < N; i++) {
    c[i] = a[i] + b[i];
}
```



- ▶ MPI\_Send
- ▶ MPI\_Recv
- ▶ MPI\_Bcast
- ▶ MPI\_Reduce

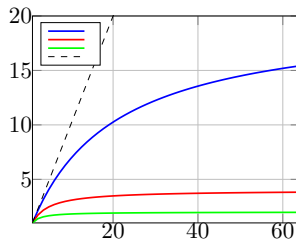






$$S(n) = \frac{1}{(1-p) + \frac{p}{n}}$$

- ▶  $S(n)n$
- ▶  $p$
- ▶  $(1-p)$





```
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"
```

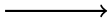
```
echo "Total tasks: $SLURM_NTASKS"
```


```
#!/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
```

```
# 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



```
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
```

```
#!/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 Distributed

addprocs(4) # Add 4 workers

@everywhere function compute(x)
```

```
using MPI

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

```
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
```

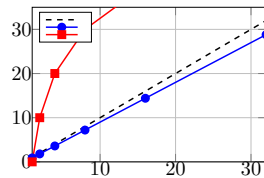
```
# Get cores from environment
ncores <- as.integer(Sys.getenv("R_NCORES", "1"))

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











sbatch

queue

- ▶  $\sum_{i=1}^N i^2$
- ▶
- ▶





sinfo

sacct--mem

--time

module availmodule load



▶ sallocsrn



▶ `/usr/bin/time -v`



▶  $= \times \times 1.3$



▶  $T \approx \frac{T}{N_{\times}}$







%j



▶ <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/>

▶ `gprofperfiIntel VTune`

▶ `gdbvalgrindDDT`

▶ `squeuesacctcontrol`

