

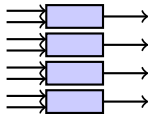






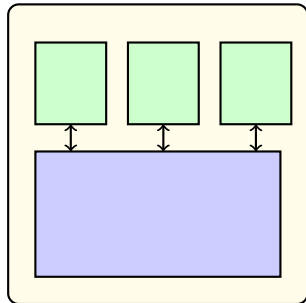


$$C[0 : 3] = A[0 : 3] + B[0 : 3]$$





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



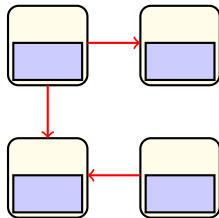


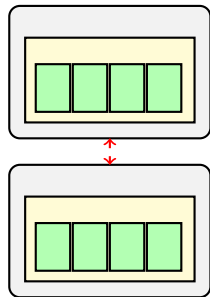
▶ MPI_Send

▶ MPI_Recv

▶ MPI_Bcast

▶ MPI_Reduce





$$S = \frac{T}{T}$$

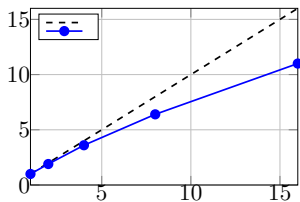
$$E = \frac{S}{N} = \frac{T}{N \times T}$$

$$E = 1$$

$$E = 0.7 - 0.9$$

$$S = 100/30 = 3.33$$

$$E = 3.33/4 = 0.83$$





N

▶ $(1 - p) \times T$

▶ $\frac{p \times T}{N}$

▶ $(1 - p) \times T + \frac{p \times T}{N}$

T

p

$(1 - p)$

$$S(N) = \frac{T}{(1 - p) \times T + \frac{p \times T}{N}}$$

T

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

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

► $S(n)n$

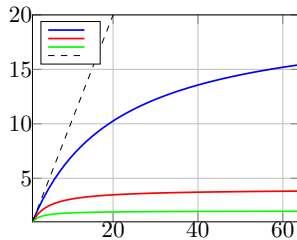
► p

► $(1-p)$

►

► $n \rightarrow \infty S \rightarrow \frac{1}{1-p}$

►





```
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`


```
#!/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"

./my_openmp_program
```

```
#!/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"

mpirun ./my_mpi_program
```

```
#!/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"
echo "OpenMP threads per task: $OMP_NUM_THREADS"

mpirun ./my_hybrid_program
```

```
--ntasks=1  
--cpus-per-task=1  
--ntasks=1  
--cpus-per-task=N  
--ntasks=N  
--cpus-per-task=1  
--ntasks=M  
--cpus-per-task=N
```



```
#!/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
- ▶ %a
- ▶ \$SLURM_ARRAY_TASK_ID

- ▶ --array=1-100
- ▶ --array=1-100:10
- ▶ --array=1,5,10,15
- ▶ --array=1-100%10

▶

▶

▶

```
# 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, run multiple commands
hostname
module load python
python # Interactive Python session
# ... work interactively ...
exit # Release resources when done
```

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 ex:
    results = ex.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
```

```
# In Python script
import os
from multiprocessing import cpu_count
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

# Test
arr = rand(1000000)
total = parallel_sum(arr)
```

```
#!/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
```



▶ @threads



```
using Distributed

# Add 4 worker processes
addprocs(4)

# Function available on all workers
@everywhere function compute(x)
    return x^2
end

# Parallel reduction
results = @distributed (+) for i = 1:100
    compute(i)
end

println("Sum of squares: $results")
```

```
using MPI

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

# Each rank does work
local_result = rank * 10

# Gather results
all_results = MPI.Gather(
    local_result, 0, comm)

if rank == 0
    println("Results: $all_results")
end
```

```
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()

# Parallel apply
results <- mclapply(
  1:100,
  function(x) x^2,
  mc.cores = ncores)

# Convert to vector
results <- unlist(results)
```

`mclapplyforeach`

```
#!/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"))

# Use with foreach
cl <- makeCluster(ncores)
registerDoParallel(cl)

# ... rest of code ...

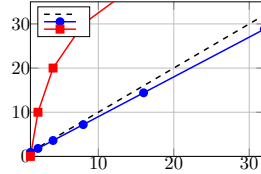
stopCluster(cl)
```



▶ .combine









sbatch

queue

- ▶ $\sum_{i=1}^N i^2$
- ▶
- ▶




```
sinfo  
sacct--mem--mem-per-cpu  
--time  
scontrol show partition
```



▶ sstat

▶ sacct

```
module availmodule load
```

```
$SLURM_SUBMIT_DIR
```



echo

- ▶ `stderr`



- ▶ `sallocsrun`



▶ `/usr/bin/time -v`



▶ $= \times \times 1.3$



▶ $T \approx \frac{T}{N_{\times}}$





▶ %j



▶ `squeue -u $USER`

▶ `sacct`

▶ `sstat`







▶ <https://slurm.schedmd.com/>



▶ `man sbatchman srun`

▶ <https://www.hpc-carpenentry.org/>

▶ <https://www.xsede.org/for-users/training>

▶ <https://www.openmp.org/resources/tutorials-articles/>

▶ <https://mpitutorial.com/>

▶ `gprofperfl Intel VTune`



`llnl -l -i -l DDT`

