

◦ Parallelization (cont. from last time)

◦ Recap:

- Two approaches: Shared memory (e.g. OpenMP)
Distributed memory (e.g. MPI)

◦ [Go through OpenMP examples in the Git repo]

◦ Different approaches to parallelize project 4:

Alt 1) Parallelize loop over temperatures (simplest!)

Alt 2) For each temp., use parallelization to run multiple MCMC chains (multiple "walkers")
Can either:

- Increase number of threads and decrease cycles per thread

Each walker/chain needs burn-in

or:

⇒ same accuracy, shorter time

- Increase number of threads while keeping number of cycles per thread fixed

⇒ higher accuracy (more MC samples), same time

Alt 3) For each temperature and each MC cycle, parallelize the "sweep" over the spin matrix

- Most complicated! (Don't do this...)
- Most overhead

- How to define speedup from parallelization

$$\text{Speedup} = \frac{\text{time with single thread/process}}{\text{time with } n \text{ threads/processes}} = \frac{T_1}{T_n}$$

- Ideal case: n threads $\Leftrightarrow T_n = \frac{T_1}{n} \Leftrightarrow$ speedup factor is n

- In most cases we will not get ideal speedup
- In rare cases we can get better than ideal speedup (e.g. through changes in memory access)

- Keep in mind: A complicated algorithm with less than ideal speedup from parallelization can still be a better choice than a simple algorithm with better (ideal?) parallelization speedup!

- Example: Find the maximum of a complicated, high-dim function through

1) random sampling (ideal speedup, "embarrassingly parallelizable") or grid scan

2) sophisticated optimization algorithm, e.g. differential evolution

[show example from paper]

(needs communication and synchronization \rightarrow less than ideal speedup)

◦ Upper bound on speedup :

- A task takes time T_1 on single thread/process

→ Fraction of time spent in perfectly parallelizable code : f

→ Non-parallelizable fraction : $1-f$

◦ Single thread/process :

$$T_1 = (1-f)T_1 + fT_1$$

◦ On n threads/processes :

$$T_n = (1-f)T_1 + f \frac{T_1}{n}$$

◦ Speedup :

$$\frac{T_1}{T_n} = \frac{T_1}{(1-f)T_1 + f \frac{T_1}{n}} = \frac{1}{(1-f) + \frac{f}{n}}$$

$$\lim_{n \rightarrow \infty} \frac{T_1}{T_n} = \frac{1}{1-f}$$

Amdahl's law

Examples: If 99% of a task is parallelizable ($f=0.99$)
the maximum possible speedup factor
is $\frac{1}{1-0.99} = \frac{1}{0.01} = 100$

Example 2 : $f = 0.80 \Rightarrow$ max speedup is 5