Intro to Multithreading

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Applied Math 205
Harvard University

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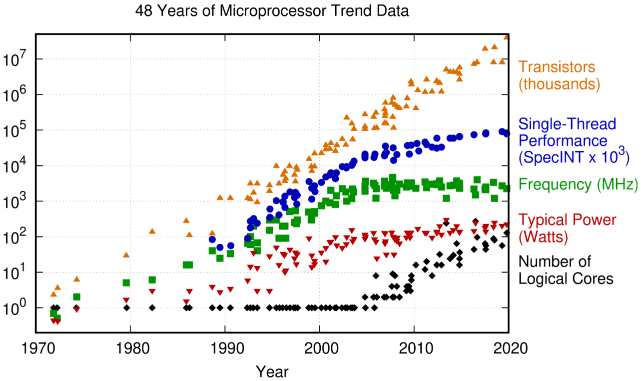
The processor (CPU/central processing unit) is the collection of circuitry which executes the instructions making up a computer program.

CPU clock speeds have stagnated since the mid-2000s. Hardware improvements have come in the form of more cores per CPU.



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
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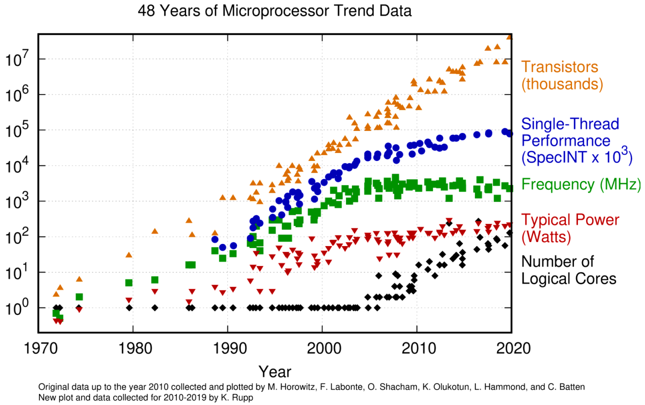

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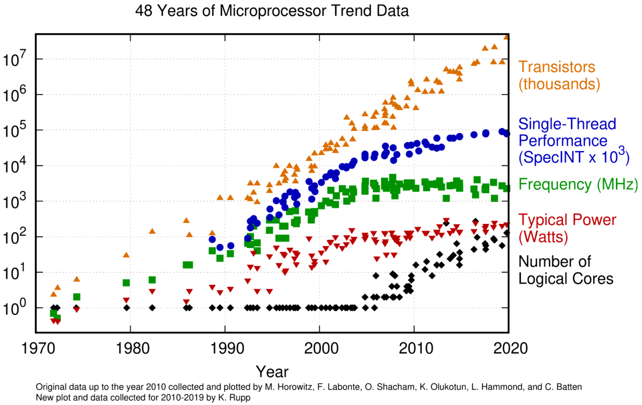

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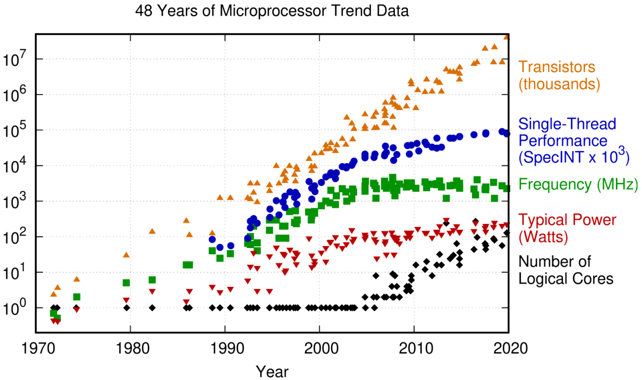

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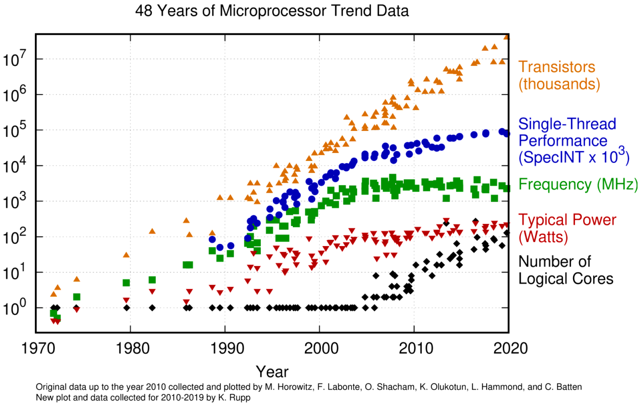

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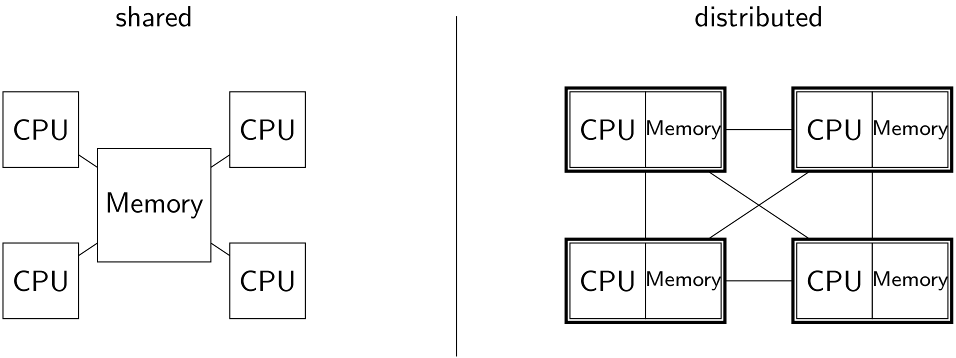
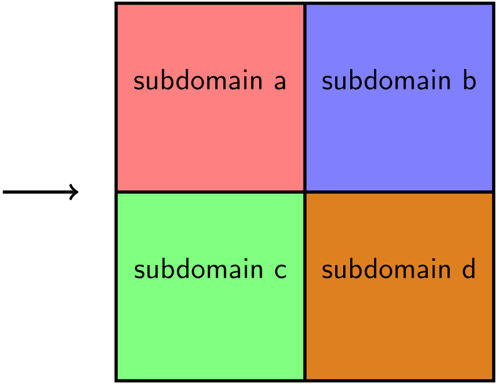
- faster clock speeds $\implies$ higher power
- more cores + slower clock speeds can yield **higher** compute power with **lower** power consumption
- higher core counts are becoming more and more widely available
- important to understand how to adapt or write code to take advantage of parallel architecture

There are two main paradigms of code parallelization: shared memory and distributed memory.



Programs parallelized with distributed memory run as several independent threads, pausing only to periodically communicate amongst each other.

One method of memory distribution is to divy up the **simulation domain** across the various threads.



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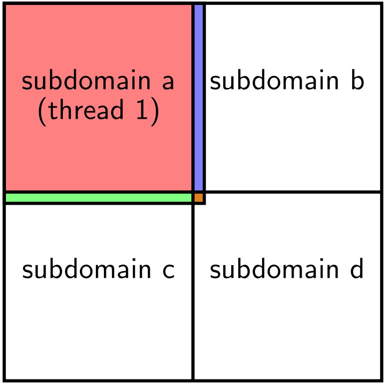

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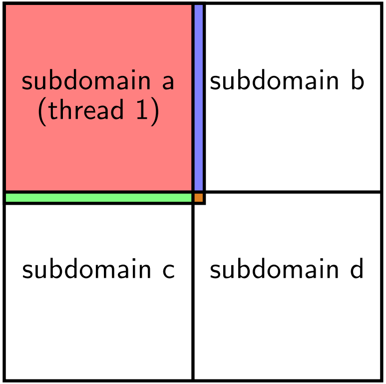

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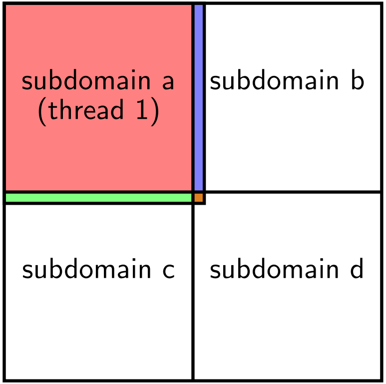
  $\Longrightarrow$ need **communication**

  b, c, d send to a



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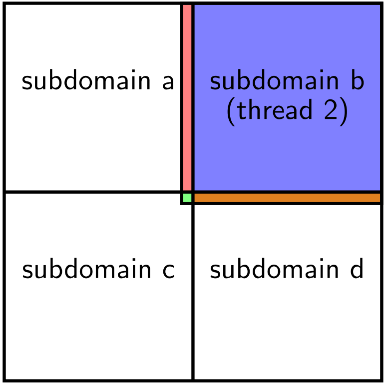

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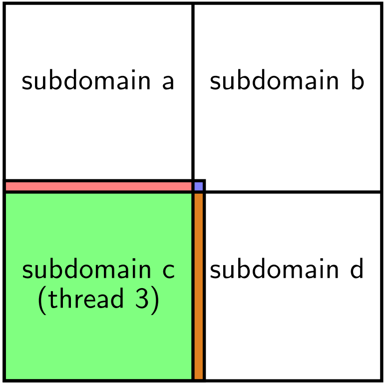

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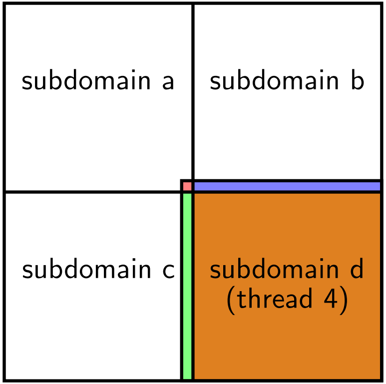

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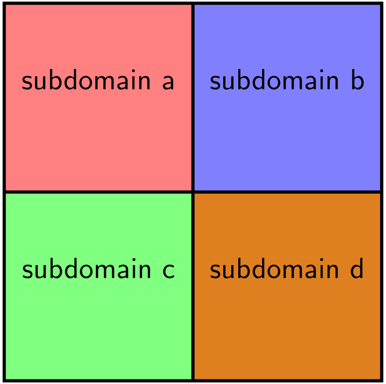

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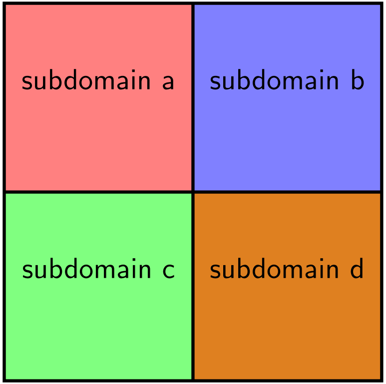

Discuss: benefits? costs?

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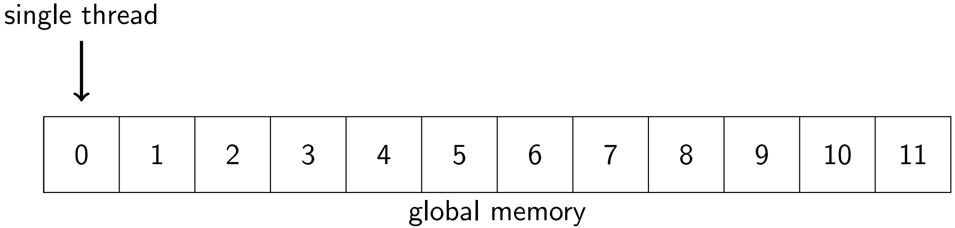
A single thread loops sequentially through each spot in memory



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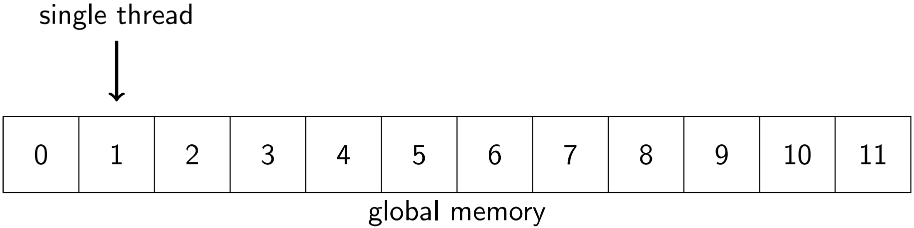

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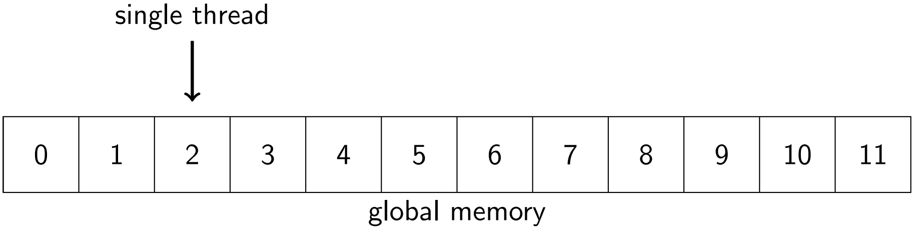

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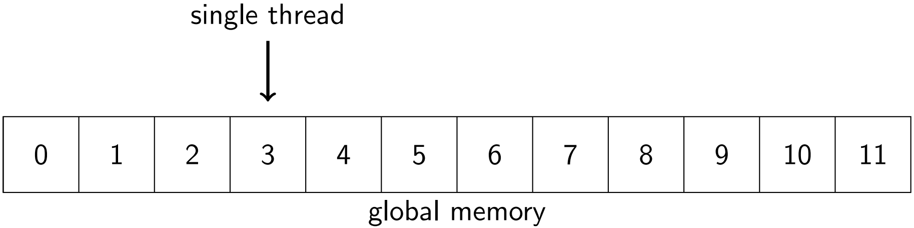

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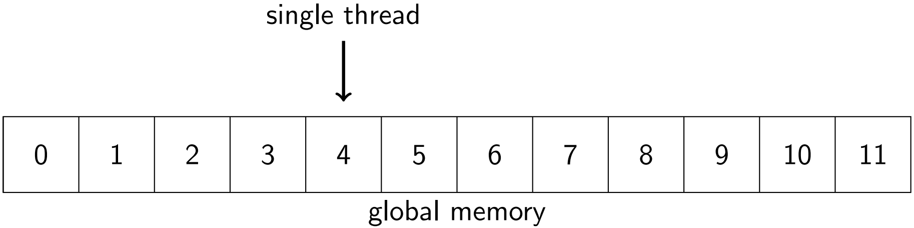

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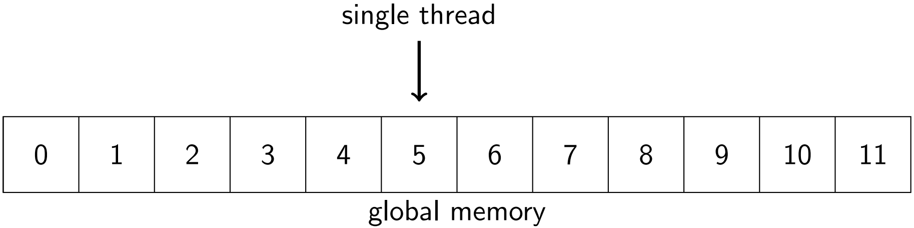

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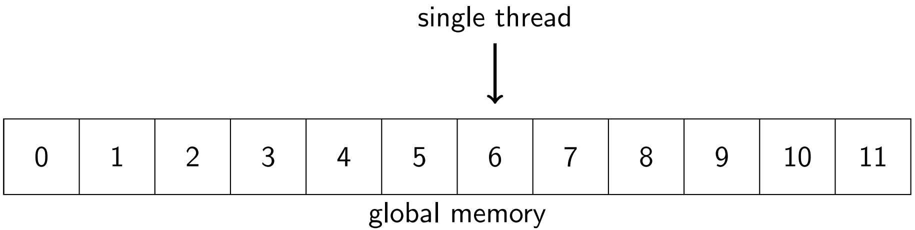

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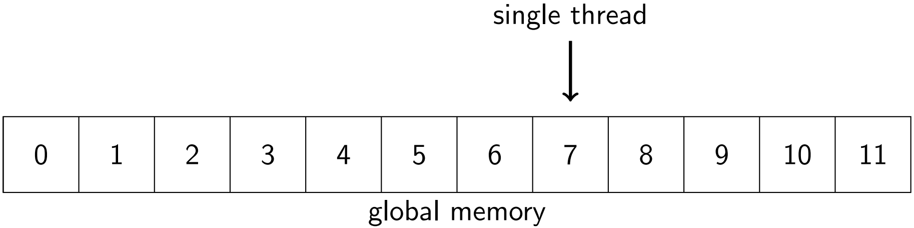

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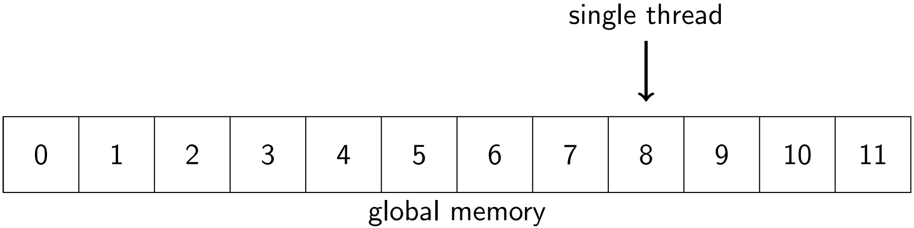

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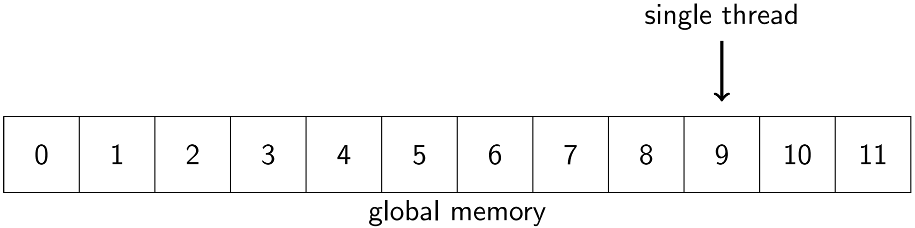

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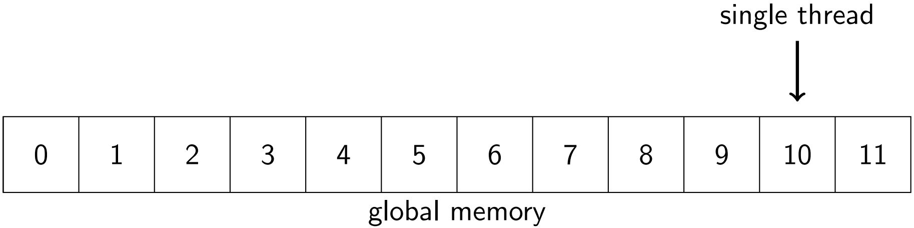

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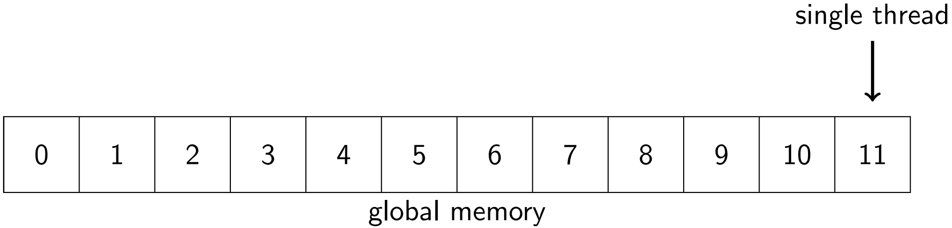

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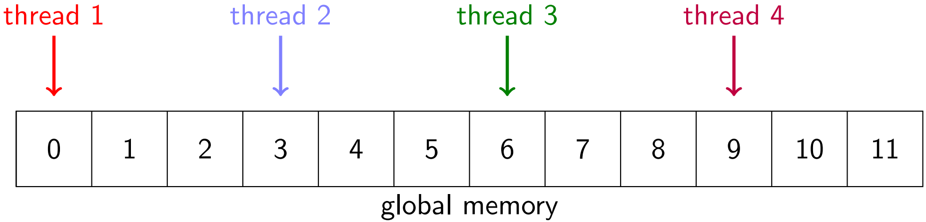

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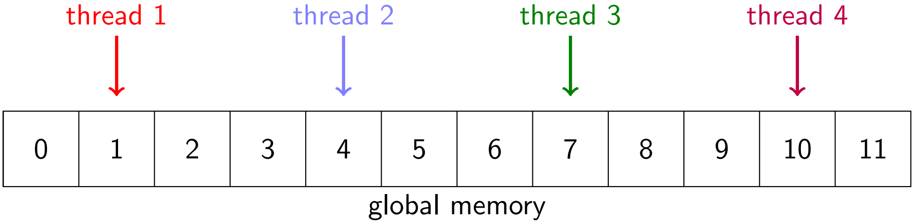

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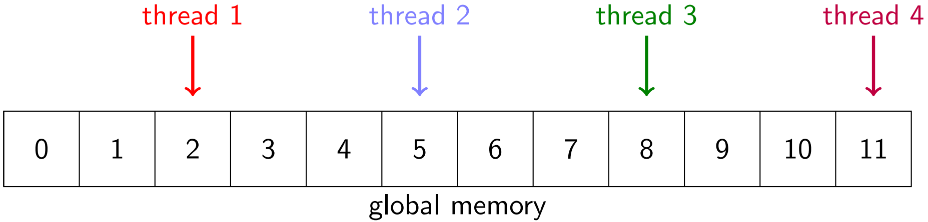

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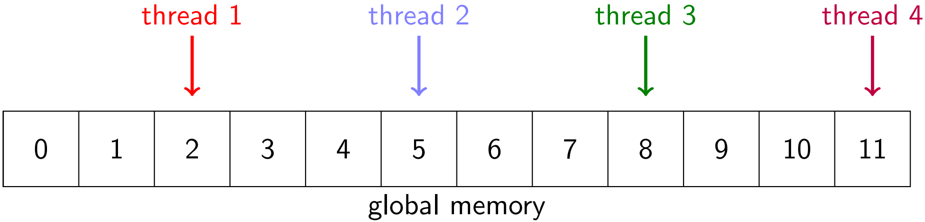

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- overhead for k threads $\propto k$
- as k grows, $k > N$ (threading becomes bigger job than original goal)
- as N grows, problem may become memory bandwidth-limited (implementation-dependent)

In C++, shared-memory parallelization can be implemented with the OpenMP API.

Anatomy of an OMP call:

```
// add two vectors of length N
static const int N=10;
double v1[N],v2[N],v3[N];

#pragma omp parallel for
for (int i=0; i<N; i++) {
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$\Longrightarrow$ no one iteration depends on another! “embarrassingly parallel”

Explicit precautions must be taken if multiple threads are writing to one location in memory or a value is being calculated across multiple threads.

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// dot product (method 1)
double dot=0;
#pragma omp parallel for shared(dot)
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- mark dot as a shared variable among all threads (this is actually the default behavior)

Explicit precautions must be taken if multiple threads are writing to one location in memory or a value is being calculated across multiple threads.

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// dot product (method 1)
double dot=0;
#pragma omp parallel for shared(dot)
for (int i=0; i<N; i++) {

#pragma omp atomic
    dot += v1[i] * v2[i];
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OMP is not smart enough to avoid multiple threads reading/writing to the same location at the same time ("race condition"). You have to help it!

Explicit precautions must be taken if multiple threads are writing to one location in memory or a value is being calculated across multiple threads.

A better way:

```
// dot product (method 2)
double dot = 0;
#pragma omp parallel for reduction(+:dot)
for (int i=0; i<N; i++) {
    dot += v1[i] * v2[i];
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All roads lead to Rome, but some get there faster.

OMP calls allow for other specifications as well, including number of threads, private vs. shared variable defaults, scheduling, etc.

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int nt=4;
double x,y;
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Let's look at OMP in action.

We can also divide up embarassingly parallel for loops using Python using `joblib`, a wrapper for the `multiprocessing` module.

Anatomy of an joblib call:

```
import joblib as jl

# function for sum of ith components
def sum(i):
  global v1
  global v2
  return v1[i] + v2[i]

# generator of functs and args
fgen = (jl.delayed(sum)(i)
                for i in range(len(v1)))

# parallel sum
v3 = jl.Parallel(n_jobs=NUM_THREADS)(fgen)
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- Parallel object takes in args (e.g. n_jobs) and generator, returns array with result of passed function at each spot in loop

For loops—and therefore the spawning of parallel threads—take place at a higher level in Python, so there is a much higher overhead cost.

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Discuss: what properties make a job more (or less) appropriate for joblib?

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Often, modules such as numpy already have precompiled code which is parallelized
$\implies$ you don't have to do it yourself! Write **vectorized code**.

Vectorization refers to code with "invisible" for loops.

For two numpy arrays `a` and `b`, we can do the same calculation with an explicit for loop or vectorized numpy functions that call precompiled C++-code.

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for i in range(len(a)):
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c = a + b
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- dot product

```
d = 0
for i in range(len(a)):
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```

```
d = a.dot(b)
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- dot product

```
d = 0
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```

```
d = a.dot(b)
```

- elementwise multiply

```
for i in range(len(a)):
    c[i] = a[i] * b[i]
```

```
c = a * b
```

Vectorized code is faster first and foremost because of precompiled library functions, but these libraries are often parallelized with OpenMP as well.

$\boxed{\texttt{M.dot(v)}}$

(numpy code)

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(numpy code) (interpreter call)

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`M.dot(v)` ⟶

```
#pragma omp parallel for
for (int r=0;r<N;r++) {
    for (int c=0;c<N;c++) {
        out[r] += M[r][c] * v[c];
    }
}
```

(numpy code) (interpreter call) (machine code equivalent to above, compiled)

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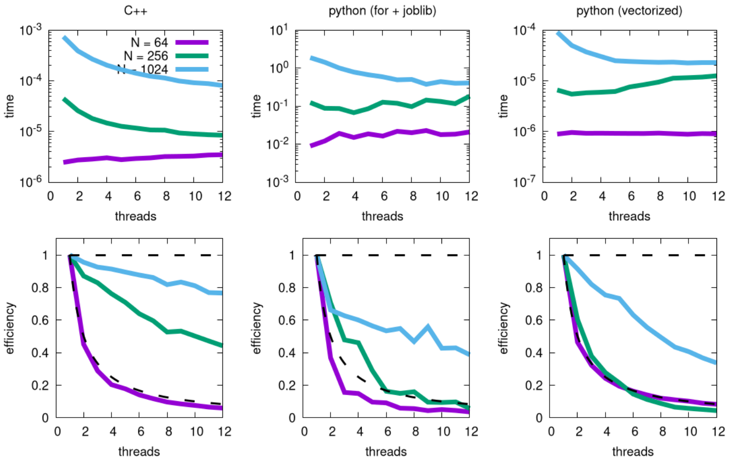
Easiest way to set thread number for vectorized `numpy`? `OMP_NUM_THREADS` environment variable!

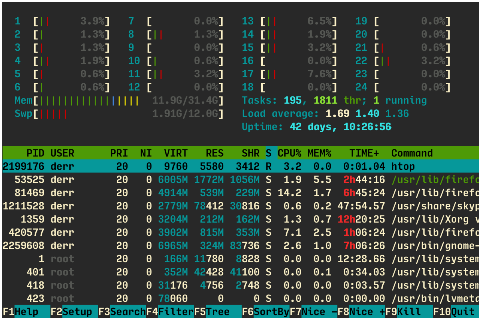
We can compare the parallel results across C++ (OMP), Python (joblib), and Python (vectorized) for a matrix multiplication



“Hyperthreading” refers to a CPU managing two sets of tasks per core.

I have 12 cores, `htop` reports 24: use them all?

answer: maybe



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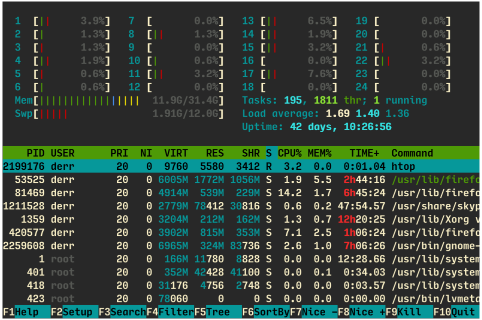

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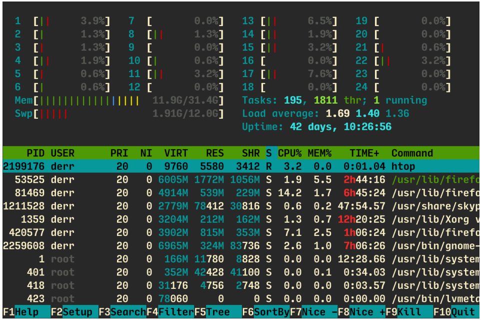

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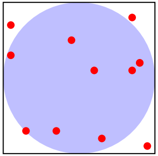
if loop iterations have dead time (can happen with very short iteration tasks), hyperthreading may allow for faster simulation time (with lower efficiency than adding more physical cores)

Summary

- Shared vs. distributed memory: use the paradigm appropriate for your problem
- Compiled languages
  - want a speed up? find main for loop, drop in `#pragma omp parallel for`
  - threads will do what you tell them to do: **be careful!** Use OMP options
  - compiler flexibility (multithreaded code works on non-OMP compilers)
- Interpreted languages
  - parallelization often include by default in calls to precompiled library functions
  - eschew for loops: **vectorize, vectorize, vectorize**
  - help your CPU out in determining number of threads vs. cores

Group activity: calculating π stochastically

Consider a square of area 4 inscribed with a circle of radius 1:



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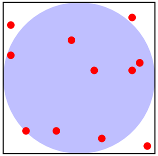

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$$f = \frac{A_{\text{circle}}}{A_{\text{square}}} = \frac{\pi}{4} \implies \boxed{\pi = 4f.}$$

Idea: generate random points, calculate approximation to π based on fraction in circle.

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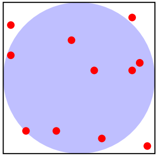

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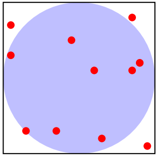

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...but how to generate an estimate for the accuracy of our approximation?

$\rightarrow$ generate N values p_i, $0 <= i < N$, from N batches of k points:

$$\boxed{\text{approx value } \bar{\pi} = \text{mean}(p_i), \qquad \text{standard error } \sigma_\pi = \frac{\text{std}(p_i)}{\sqrt{N}}}$$

Problem specification

- Using C++ and OMP, Python and joblib, or vectorized numpy, write a program that takes in integers N, k and t, with
  - N: number of π approximations
  - k: number of points generated for each π approximation
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  3. Given the above, for what types of values of N and k is multithreading most appropriate? Do your results reflect this?