Introduction to Parallel Programming

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ORCD at MIT

ORCD Overview

- Who are we?
  - Long history of supporting the computational and data needs of MIT
  - Official office status launched in September 2022
- What do we provide?
  - Sizable, shared base computing and data resources and services
  - Training and support
  - Additional direct charge services
    - Purchasing and hosting compute resources
    - Storage

+off campus operations and remote support team

https://orcd.mit.edu

Outline of the course

Day 1

- Preliminary parallel programming
- OpenMP programming
- MPI programming

Day 2

- GPU basics
- CUDA programming
- Parallel and distributed deep learning

Preliminary Parallel Programming

Outline

- Basics of HPC
- Access to ORCD clusters
- Optimize serial programs
- Embarrassingly parallel
- Parallel computing: shared memory *vs.* distributed memory

What is HPC?

- High Performance Computing (HPC) refers to the practice of aggregating computing power in order to solve large problems in science, engineering, or business.
- Similar terminology: supercomputing.
- The purpose of HPC: accelerate computer programs and thus accelerate work processes.
- HPC cluster: A set of connected computers that work together. Computers are connected with high-speed network. They can be viewed as a single system.

- Parallel computing: many computations are carried out simultaneously, typically computed on a computer cluster.
- Parallel programming: MPI, OpenMP, CUDA.

General-purpose HPC

- More and more non-traditional HPC workloads.
- Artificial intelligence (AI) training as well as compute and data-driven analytics.
- Computational demands of deep learning applications: GPUs, large memory, fast I/O.
- General-purpose HPC refers to any applications designed to run a given workload as fast as the hardware will allow. The hardware stack can be CPU, memory, storage, network, GPU, PCI, a single node, or multiple nodes on a computer cluster.

- “The convergence of AI, data analytics and traditional simulation will result in systems with broader capabilities and configurability as well as cross pollination.” -- Dr. Al Gara, Intel

Reference: https://hpcng.org/

Basic structure of an HPC cluster

- Cluster – a collection of many computers/nodes.
- Rack – a closet to hold a bunch of nodes.
- Node – a computer (with processors, memory, hard drive, etc.)
- Socket/processor – one multi-core processor.
- Core/processor – one processing unit.
- Hyperthread: virtual (logical) core

- Network devices
- Storage system
- Power supply system
- Cooling system

Computer Clusters in MGHPCC

Inside a node

- CPU (e.g. multi-core processors)

  To carry out program instructions. Built-in cache (fast memory).

- Memory (RAM)

  Fast but temporary storage, to store data for immediate use.

- Hard drives

  Relatively slow but permanent storage, to store data permanently.

- Network devices (e.g. Ethernet, Infiniband)

  To transfer data between nodes or between sites.

- Accelerator (e.g. GPU)

  To accelerate programs with parallel computing techniques.

Parallel programming languages

- C, Fortran

  Compiling languages for performance, widely used in scientific computing for decades

  Parallel library/protocol/platform: OpenMP, MPI, CUDA
- C++

  Object-oriented design is not suitable for parallel programming.
- Python

  High-level scripting languages for easy use. Call precompiled C libraries for performance.

  Parallel packages: Numpy, Multiprocessing, MPI4py, CuPy
- Julia

  Compiled for performance. Used as a scripting language.
- MATLAB

  Convenient to deal with matrices. Parallel toolbox. Parallel server.

Access to ORCD clusters

- Get started: https://orcd-docs.mit.edu/getting-started/
- Log in Engaging

```
ssh <user>@eofe10.mit.edu
```

- Work on CPUs

```
srun -t 120 -p mit_normal -N 1 -n 8 --mem=20GB --pty bash
module load gcc/12.2.0
module load openmpi/4.1.4
```

- Work on GPUs

```
srun -t 120 -p mit_normal_gpu -N 1 -n 2 --mem=10GB --gres=gpu:1 --pty bash
module load cuda/12.4.0
```

Optimize serial programs

- Before parallelization, serial programs can be optimized and thus accelerated substantially!
- Compiler optimizations

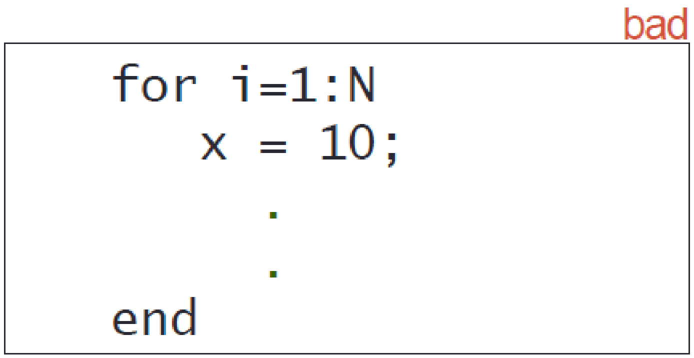
```
gcc -O3 my_code.c -o my_program
gfortran -O3 my_code.c -o my_program
```

```
icc -fast my_code.c -o my_program
ifort -fast my_code.c -o my_program
```

- Optimizing serial codes to speed up

Unnecessary work (1): redundant operations

- Avoid redundant operations in loops



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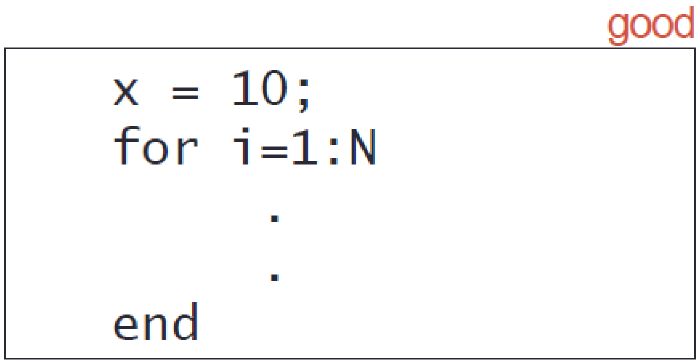
```
for i=1:N
   x = 10;
     .
     .
end
```



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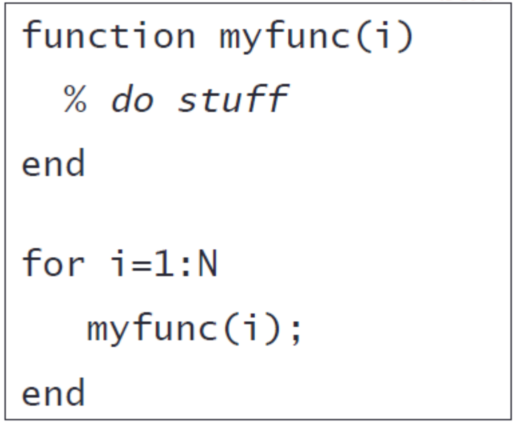
```
x = 10;
for i=1:N
     .
     .
end
```

Unnecessary work (2): reduce overhead

..from function calls

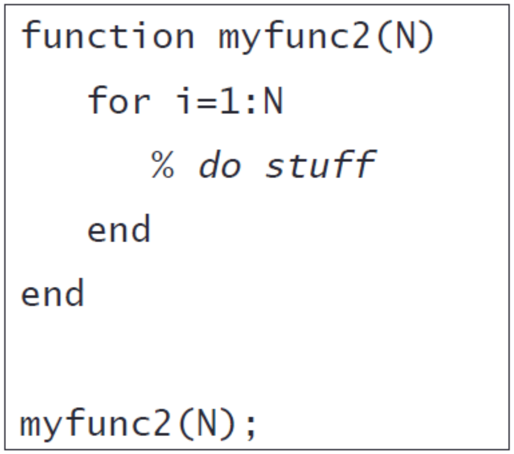
bad



```
function myfunc(i)
  % do stuff
end

for i=1:N
   myfunc(i);
end
```

good

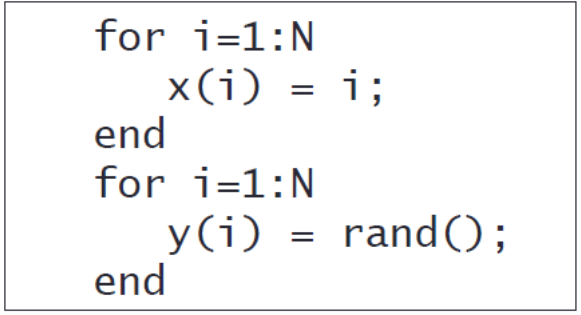


```
function myfunc2(N)
   for i=1:N
      % do stuff
   end
end


myfunc2(N);
```

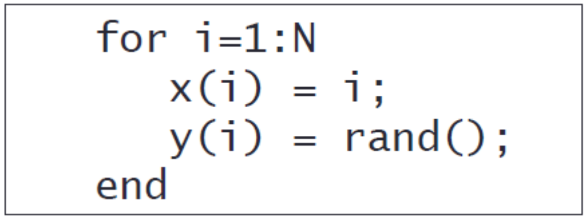
..from loops

bad



```
for i=1:N
   x(i) = i;
end
for i=1:N
   y(i) = rand();
end
```

good



```
for i=1:N
   x(i) = i;
   y(i) = rand();
end
```

Unnecessary work (3): logical tests

Avoid unnecessary logical tests...

...by using short-circuit
logical operators

bad

```
if (i == 1 | j == 2) & k == 5
   % do something
end
```

good

```
if (i == 1 || j == 2) && k == 5
   % do something
end
```

...by moving known cases
out of loops

bad

```
for i=1:N
   if i == 1
      % i=1 case
   else
      % i>1 case
   end
end
```

good

```
% i=1 case
for i=2:N
      % i>1 case
end
```

Unnecessary work (4): reorganize equations

Reorganize equations to use fewer or more efficient operators

Basic operators have different speeds:

Add	3- 6 cycles
Multiply	4- 8 cycles
Divide	32-45 cycles
Power, etc	(worse)

bad

```
c = 4;
for i=1:N
   x(i)=y(i)/c;
   v(i) = x(i) + x(i)^2 + x(i)^3;
   z(i) = log(x(i)) * log(y(i));
end
```

good

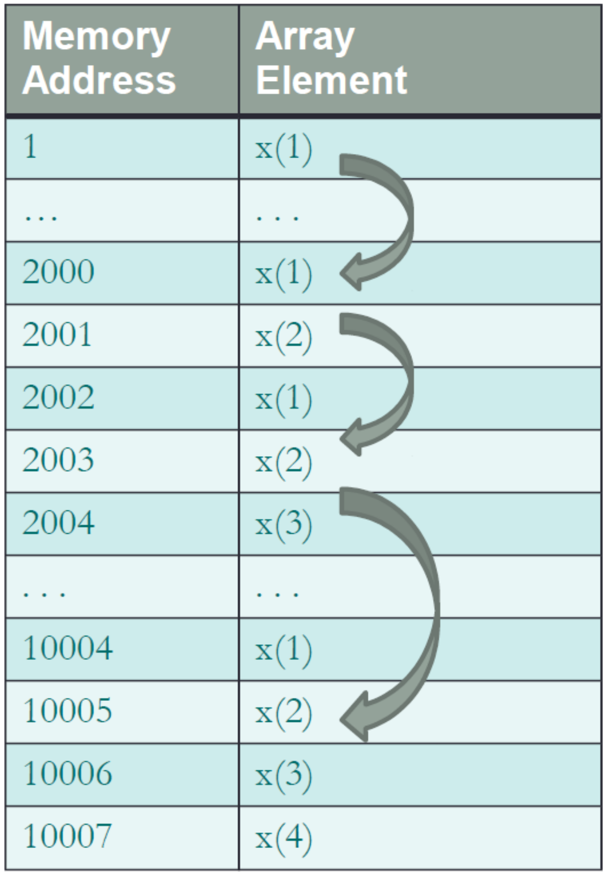
```
s = 1/4;
for i=1:N
   x(i) = y(i)*s;
   v(i) = x(i)*(1+x(i)*(1+x(i)));
   z(i) = log(x(i) + y(i));
end
```

Memory efficiency (1): preallocate arrays

- Arrays are always allocated in contiguous address space.
- If an array changes size, and runs out of contiguous space, it must be moved. For example,

```
x = 1;
for i = 2:4
   x(i) = i;
end
```

- This can be very very bad for performance when variables become large.



Memory Address	Array Element
1	x(1)
...	. . .
2000	x(1)
2001	x(2)
2002	x(1)
2003	x(2)
2004	x(3)
. . .	. . .
10004	x(1)
10005	x(2)
10006	x(3)
10007	x(4)

Memory efficiency (1): preallocate arrays

- Preallocating array to its maximum size prevents intermediate array movement and copying.

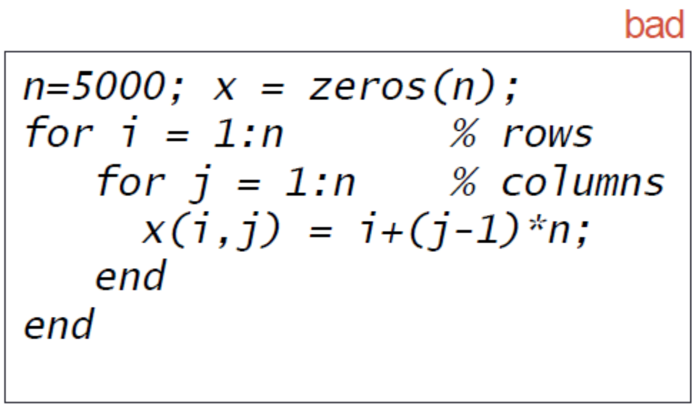
```
A = zeros(n,m); % initialize A to 0
A(n,m) = 0;     % or touch largest element
```

- If maximum size is unknown, estimate with upper bound. Remove unused memory after.

```
A=rand(100,100);
% . . .
% if final size is 60x40, remove unused portion
A(61:end,:)=[]; A(:,41:end)=[];  % delete
```

Memory efficiency (2): loop order

- It is faster to access continuous memory addresses than separated ones.
- Column-major (Fortran, MATLAB) : multidimensional arrays are stored in memory along columns.



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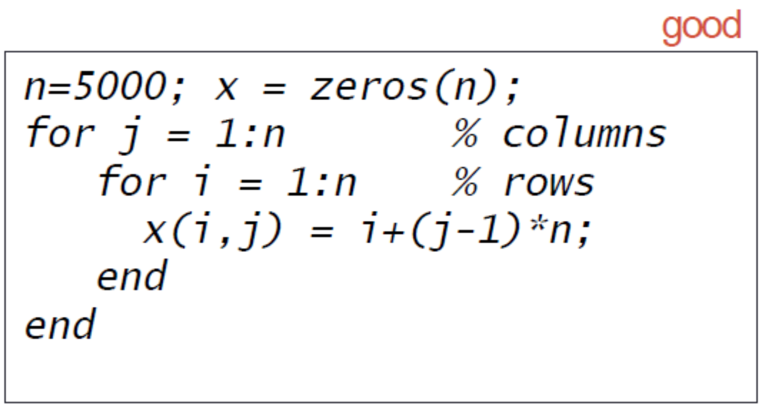
```
n=5000; x = zeros(n);
for i = 1:n         % rows
   for j = 1:n      % columns
     x(i,j) = i+(j-1)*n;
   end
end
```



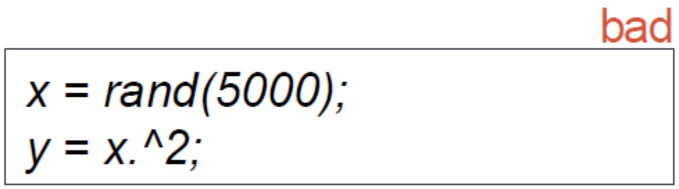
good

```
n=5000; x = zeros(n);
for j = 1:n         % columns
   for i = 1:n      % rows
     x(i,j) = i+(j-1)*n;
   end
end
```

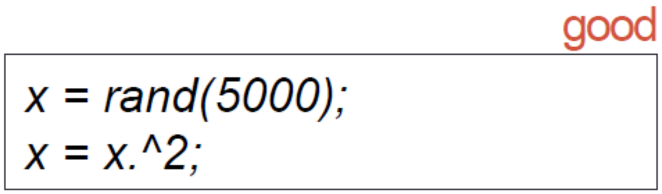
- Row-major (C, Numpy) : switch the loop order.

Memory efficiency (3): avoid unnecessary variables

- Avoid time needed to allocate and write data to main memory.
- Compute and save array in-place improves performance and reduces memory usage.



```
x = rand(5000);
y = x.^2;
```



```
x = rand(5000);
x = x.^2;
```

Embarrassingly Parallel

- Embarrassingly parallel, perfectly parallel, delightfully parallel, or pleasingly parallel.
- Run the same program with different input parameters independently
- No communications.
- Slurm job array.

Parallel Computing

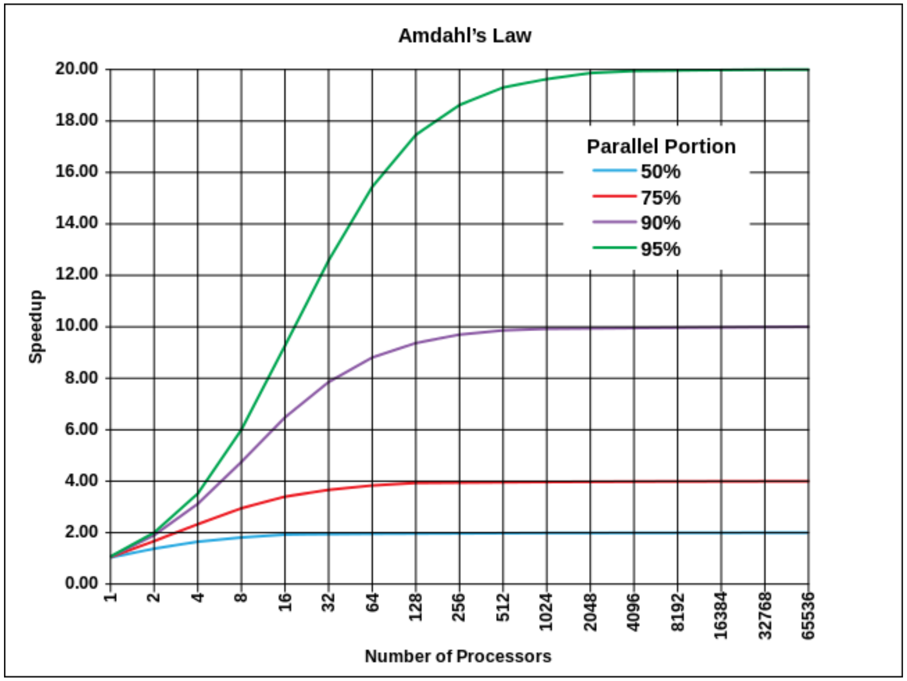
❑ Parallel computing is a type of computation in which many calculations are carried out simultaneously, based on the principle that large problems can often be divided into smaller ones, which are then solved at the same time.

❑ Speedup of a parallel program,

$$S(p) = {}^{T(1)}\!/_{T(p)} = \frac{1}{\alpha + {}^{1}\!/_{p}\,(1-\alpha)}$$

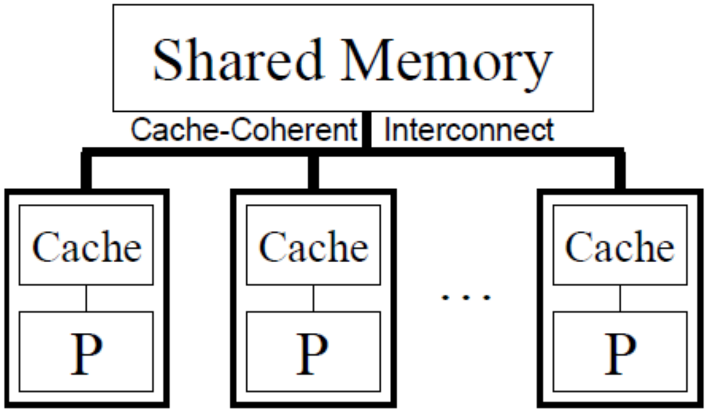
p: number of processors/cores,

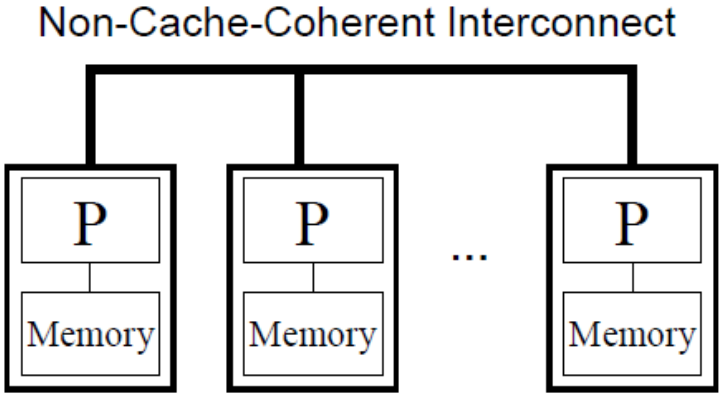
α: fraction of the program that is serial.



Ref: https://en.wikipedia.org/wiki/Parallel_computing

Distributed or shared memory systems





- Shared memory system
- Multiple cores on a single node
- Multi-processing (OpenMP, Numpy)

- Distributed memory system
- Multiple nodes on a cluster
- Message Passing Interface (MPI, MPI4Py)

MPI works on multiple cores on a node or multiple nodes.

✓ *Reference - Using OpenMP: Portable Shared Memory Parallel Programming*