MATLAB Parallel Computing Toolbox

Shaohao Chen

Research Computing Services

Information Services and Technology

Boston University

Why using Matlab Parallel Computing Toolbox (PCT)?

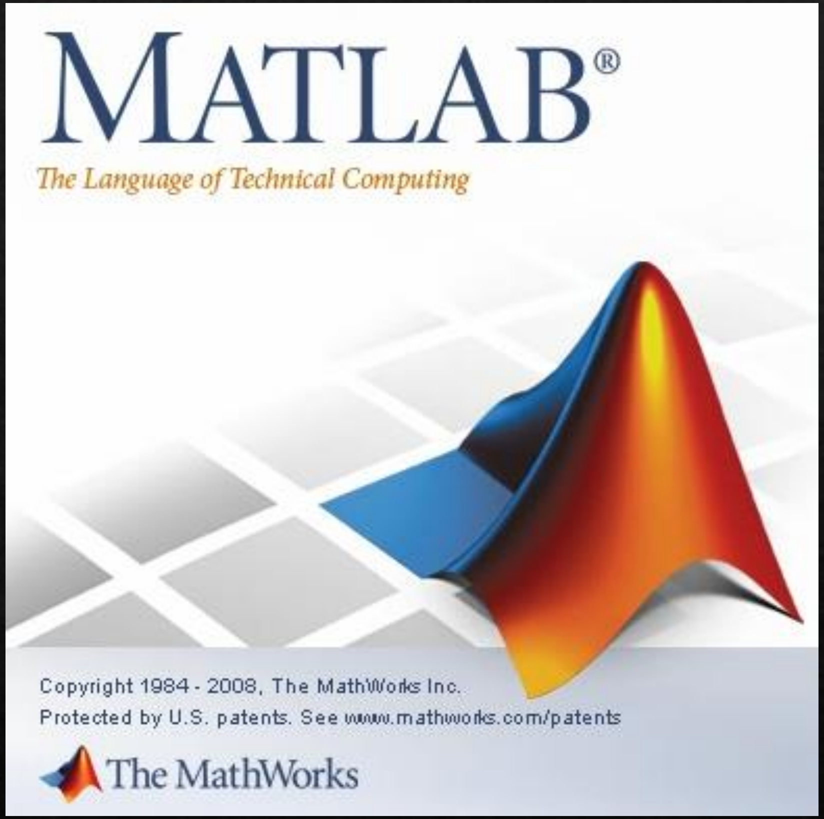
- To accelerate a MATLAB program, it is necessary to parallelize it so as to take advantages of high-performance computing (HPC) resources, such as multi-core processors, GPUs, and computer clusters.

- Boston University (BU) Shared Computing Cluster (SCC) is an HPC cluster with over 11,000 CPU processors and over 250 GPUs.
- MATLAB site license is available to all BU users. (Unlimited number on SCC).
- The PCT can be used not only on HPC clusters or but also on regular laptops/desktops.

- The skills you learn today should enable you to solve bigger problems faster using MATLAB.

Outline

- ◈ Start up MATALB on BU SCC
- ◈ Parallelize Matlab codes
- ✓ Implicit parallelism
- ✓ Explicit parallelism
- ✓ Using GPU



Access to BU SCC resources

- Log in:

$ ssh -X username@scc2.bu.edu

- Interactive session (for working interactively on compute nodes):

$ qlogin # Start an interactive session

$ qlogin -pe omp 4 # Request 4 CPU cores

$ qlogin -l gpus=1 # Request one GPU and one CPU core

- Use module to load Matlab:

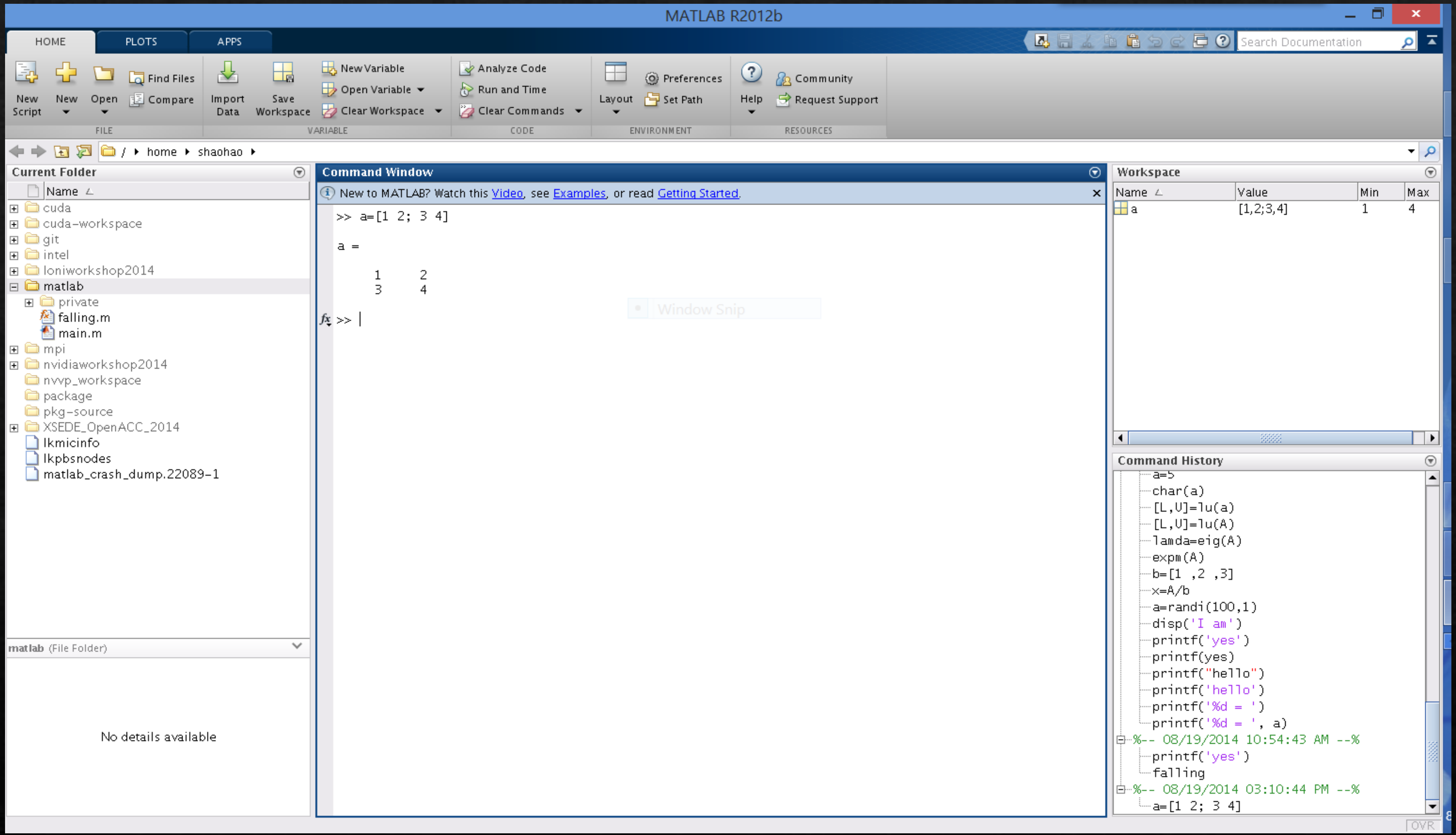
$ moduleavail | grep matlab # See all available versions

$ module load matlab # Set up environment variables

Graphic platform

- Open Matlab

$ matlab &

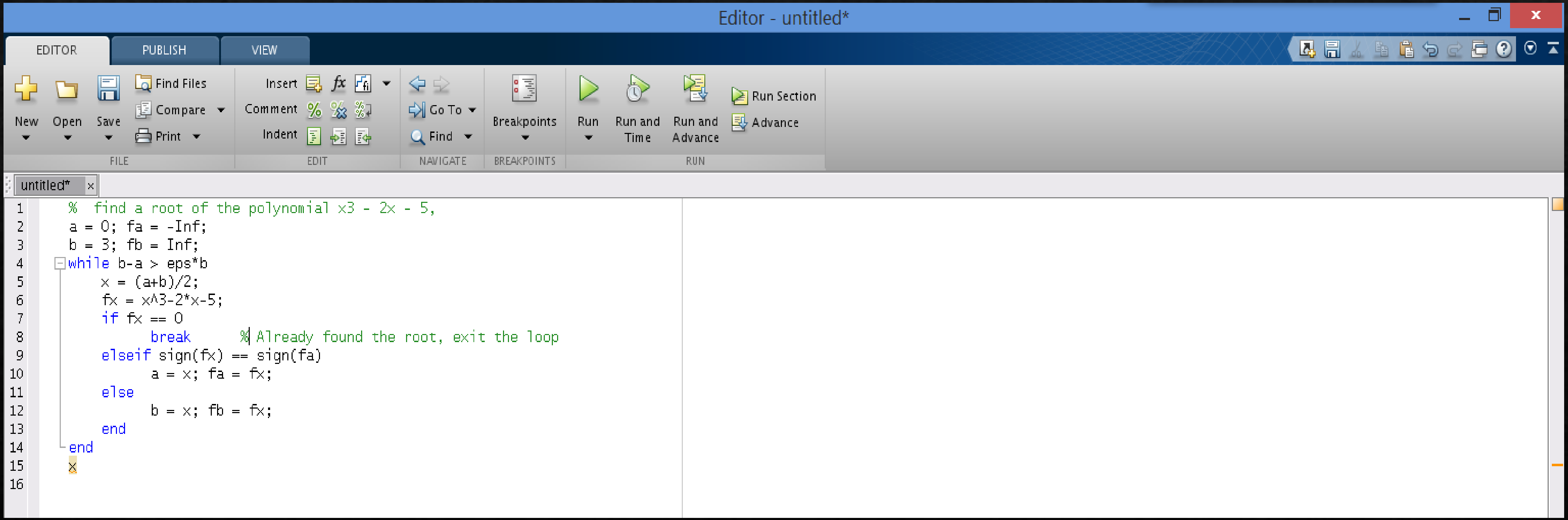


- Use VNC to speed up graphical interface.

Refer to: https://www.bu.edu/tech/support/research/system-usage/getting-started/remote-desktop-vnc/

M-file

- An m-file is a simple text file where you can place MATLAB commands.
- Save your works
- Convenient for debugging
- Run directly. Pre-compiling is unnecessary.



Text platform

$ matlab -nodisplay % Work in text interface. Does not display any graph.

$ matlab -nodesktop % Program in text interface. Pop out graphs when necessary.

- Many Linux commands (prefix an exclamation mark) are available within Matlab platform, such as:

  cd, ls, pwd, !cp, !rm, !mv, !cat, !vim, !diff, and !grep

- Edit M-file and run the program:

```
>> !vim mfilename.m      %  edit in text window
>> edit mfilename.m      %  create a new or open an existing m-file in graphical window
>> open mfilename.m      %  open an existing m-file in graphical window
>> run mfilename.m       %  run the program
>> mfilename             %  run the program
```

Parallelize Matlab codes

- Parallel computing:

  run multiple tasks by different workers simultaneously.

- Matlab parallel computing toolbox (PCT)
- ✓ Implicit parallelism: automatic multi-threaded vector operations
- ✓ Explicit parallelism: parpool, parfor, spmd
- ✓ Using GPU: gpuArray, arrayfun

Parallel Computing

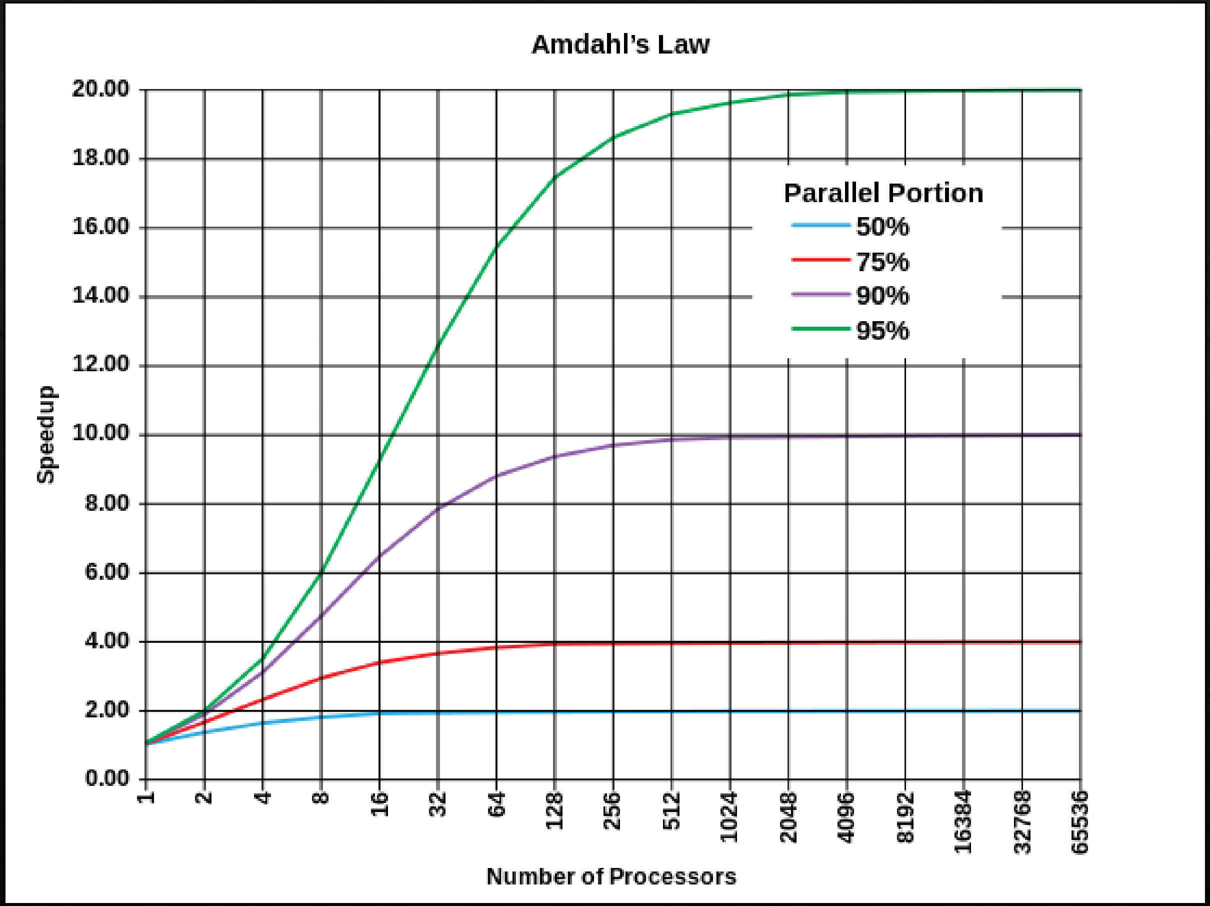
- Parallel computing is a type of computation in which many calculations are carried out simultaneously.

- Speedup of a parallel program,

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

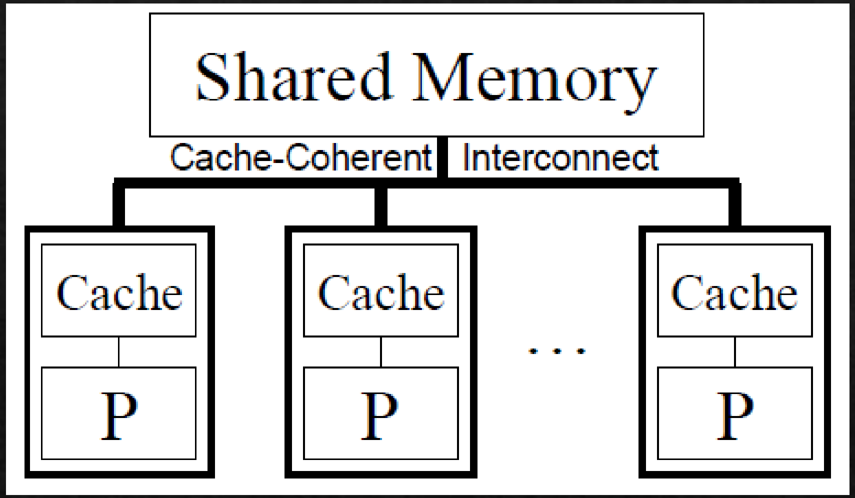
p: number of processors/cores,

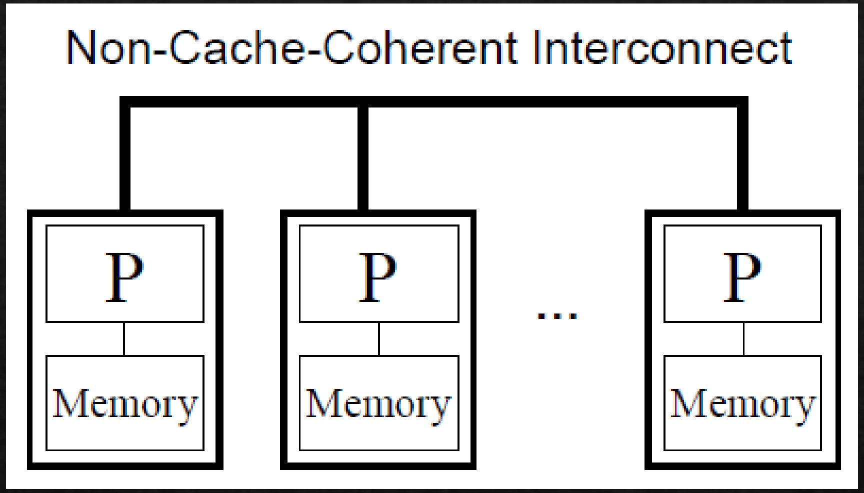
α: fraction of the program that is serial.



- Figure from: https://en.wikipedia.org/wiki/Parallel_computing

Two types of Parallel Computers





- Share memory
- Multiple CPU cores within one node

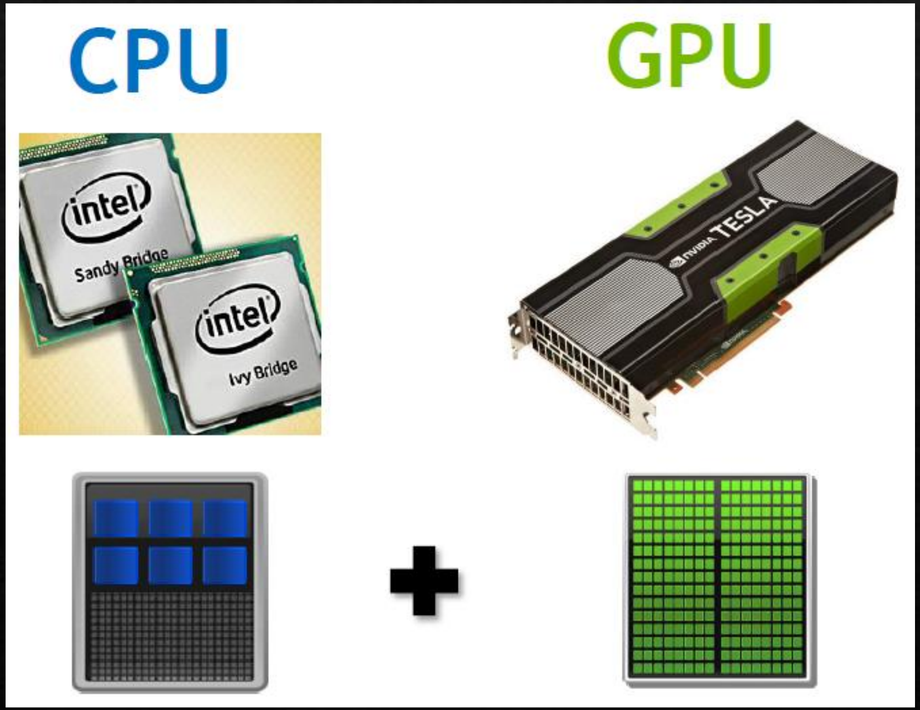
- Distribute memory
- Multiple nodes within one cluster

- Implicit (multithreaded) parallelism in Matlab is only for multiple cores on one node.
- Explicit parallelism in Matlab can be implemented on either single node or multiple nodes.

  Only the single-node mode is supported on BU SCC currently.

Graphic Processing Unit (GPU)

- GPU is a device attached to a CPU-based system.
- Computer program can be parallelized and accelerated on GPU.
- CPU and GPU has separated memory. Data transfer between CPU and GPU is required.
- GPU-enabled Matlab functions are limited but growing.



Implicit parallelism: multithreaded operations

- Many built-in operators or functions are implicitly multi-threaded, such as,

Basic operators: +, -, .*, ./, .^, *, ^, \

Basic functions: MAX, MIN, SUM, SORT

Elementary math: ATAN2, COS, CSC, SEC, SIN, TAN, EXP, POW2, SQRT, ABS, LOG, LOG10

Linear algebra: INV, LINSOLVE, LU, QR, EIG

Data analysis: FFT, CONV2

✓ Multithreading may be triggered for vector implementation but not for loop implementation.

- By default on BU SCC, these operations automatically use the requested number of CPU cores in a batch job.
- Use function maxNumCompThreads(n) to limit the number of cores to be used.

Multithreaded Matrix Multiplication

```
n=7000;
A=randn(n);   B=randn(n);     % initialize data
C=zeros(n);    D=zeros(n);

tic        %  start measuring time
C = A * B;          % multithreaded by default
toc        %  end measuring time

maxNumCompThreads(1);  % enforce using 1 thread
tic
D = A * B;       % single thread
toc
```

parpool

- parpool enables the full functionality of the parallel language features (parfor and spmd) by creating a special job on a pool of workers, and connecting the MATLAB client to the parallel pool.
- ✓ Client/master: runs serial work. Interactive with users (e.g. for input, output, serial parts).
- ✓ Workers/labs: run parallel work. Typically each worker uses one CPU core.

- Syntax

```
parpool(poolsize)
    % perform parallel works
delete(gcp)
```

- ✓ poolsize, the number of workers, is a user-defined variable.
- ✓ gcp (get current parpool) is a built-in variable.

parfor (1): Basics

- Simple: a parallel for-loop
- Work load is distributed evenly and automatically according to loop index.
- Data starts on client (base workspace), automatically copy input data to workers' workspaces, and copy output data back to client when done.
- Details are intentionally opaque to user. There are many additional restrictions as to what can and cannot be done in a parfor loop – this is the price of simplicity.

- Syntax

```
parfor i=1:n
    % Do iteration work
end
```

- An example:

```
x=zeros(1,12);
parfor i=1:12
    t = getCurrentTask(); disp(t.ID);  % Dispaly worker ID
    x(i)=10*i;   % Computation is done by workers simutaneously
end
```

parfor (2): Rules for variables

- For the parfor loop to work, variables inside the loop must all fall into one of these categories:

Type	Description
Loop	A loop index variable for arrays
Sliced	An array whose segments are manipulated on different loop iterations
Broadcast	A variable defined before the loop and is used inside the loop but never modified
Reduction	Accumulates a value across loop iterations, regardless of iteration order
Temporary	Variable created inside the loop, but not used outside the loop

parfor (3): Modify variables

```
n=12;
s = 0;
X = rand(1,n);
b = 10;
parfor k = 1 : n
    a = 2*k;         % a - temporary var; k - loop index
    Y(k) = X(k) + a*n;       % X, Y - sliced var;  n - broadcast var (not modified in the loop)
    b = 20;       % b - temporary var: the value is not carried out of the loop
    s = s + a;    % s - reduction var: : the value is carried out of the loop
end
```

parfor (4): Reduction

- Reduction variables appear on both sides of an assignment statement, such as:

  X = X *op* expr

  X = expr *op* X (except subtraction)

- ✓ The operation *op* could be +, -, *, .*, &, |

- A failed case: not a reduction:

```
x = 1;
parfor  i= 1:10
     x = i - x;
end
```

- A successful case: a reduction:

```
x = 1;
parfor  i= 1:10
     x = x - i;
end
```

parfor (5): Data dependency

- Data dependency: loop iterations must be independent

- A failed case:

```
n=10;
a = 1:n;
parfor  i= 2:n
    a(i) = a(i-1)*2;
end
% This may return unexpected results.
```

- A successful case:

```
n=10;
a = 1:n;
parfor  i= 1:n
    a(i) = a(i)*2;
end
% Each a(i) is read and modified by one worker only. Different indexes are independent.
```

parfor (6): Loop index

- Loop index must be consecutive integers.

```
parfor i= 1 : 100        % OK
parfor i= -20 : 20       % OK
parfor i= 1 : 2 : 25     % No
parfor i= -7.5 : 7.5     % No
A = [3 7 -2 6 4 -4 9 3 7];  parfor i= find(A > 0)     % No
```

parfor (7): Nested loops and functions

- The body of a parfor-loop ……
- ✓ can contain for-loops, including further nested for-loops.
- ✓ can not contain another parfor-loop.
- ✓ can make reference to a regular function but not a nested function.
- ✓ can call a function that contains another parfor-loop, which runs in parallel only if the outer parfor-loop runs serially (e.g. specifying one worker).

- Refer to: https://www.mathworks.com/help/distcomp/nesting-and-flow-in-parfor-loops.html

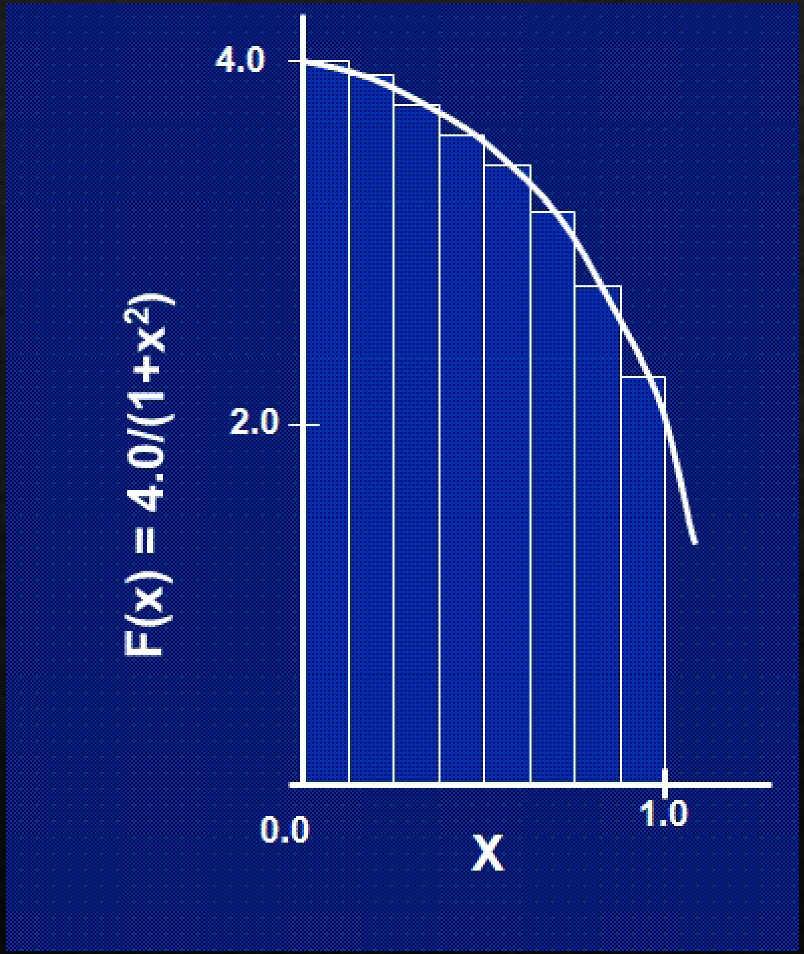
Compute the value of Pi

- Compute the value of Pi using the integral formula

$$\int_0^1 \frac{4.0}{(1+x^2)}\,dx = \pi$$

- The serial code

```
n=2000000000;  dx=1/n;   pi=0;
for i=1:n
    x = (i - 0.5) * dx;
    pi = pi + 4./(1.+x*x);
end
format long
pi=pi*dx
```



Exercise 1

- Compute the value of Pi using parfor

  i) Parallelize the code using parfor . Check whether all variables in the parfor region fall into one of the valid categories.

  ii) Compare the performances of the serial and the parallel codes.

spmd (1): Basics

- spmd = Single Program Multiple Data

Explicitly and/or automatically…

- ✓ divide work and data between workers/labs
- ✓ communicate between workers/labs

- Syntax

```
% execute on client/master out of spmd region
spmd
    % execute on all workers within spmd region
end
% execute on client/master out of spmd region
```

spmd (2): Number and index of workers

- Get an array chunk on each worker using numlabs and labindex

```
parpool(4)
spmd
   disp(numlabs);  % numlabs – total number of workers, built-in variable
   disp(labindex);  % labindex – index of workers, built-in variable
   N=24;
   A=1:2:N;
   I = find(A > N*(labindex-1)/numlabs & A <= N*labindex/numlabs)
end
delete(gcp)
```

Pmode: Interactive Parallel Command Window

- Workers receive commands entered in the Parallel Command Window, process them, and send the command output back to the Parallel Command Window.

- Launch pmode

```
>> pmode start 4   % Request 4 workers
```

- Execute commands in pmode (at prompt P>>)

```
P>> x = 2 * labindex
P>> y = numlabs
P>> if labindex == 1
        z = x*10 + y
    end
```

spmd (3): Send and receive data

- labSendReceive(ID_send_to, ID_receive_from, send_data) - Send data to one worker and receive data from another worker.
- Example: circularly shift data between neighbor workers

```
spmd
   DataSent=labindex;
   right = mod(labindex, numlabs) + 1;          % one worker to the right
   left = mod(labindex - 2, numlabs) + 1;       % one worker to the left
   % Send data to the right and receive another data from left
   DataRcv = labSendReceive(right, left, DataSent)
end
```

spmd (4): Broadcast data

- labBroadcast - Broadcast data from one worker to all other workers.

```
spmd
  source=1;
  if labindex == source
     data=1:12;
% send data from the source worker to other workers, and save it in shared_data on the source worker.
     shared_data = labBroadcast(source, data)
  else
     % receive data on other workers and save it in share_data
     shared_data = labBroadcast(source)
  end
end
```

spmd (5): Composite variable and distributed array

- Use Composite, distributed out of spmd region

```
a=5;                                      %  Create a normal variable on client
b=Composite(); c=Composite();             %  Create composite variables b and c on client
A=ones(4,4);   A=distributed(A);          %  Create a matrix A on client and distribute it to workers
spmd
   x = a          %  Variable a is copied to workers and assigned to x. The local variable x is not accessible from client.
   y = labindex       % Variable y is a local variable and is not accessible from client.
   b = labindex;      % Composite variable b is modified by workers and is accessible from client
   c = magic(labindex+2);        % Composite variable can be a matrix too.
   B = A * 2;          % Computation is distributed to workers. The result matrix B is accessible from client.
end
b{:}    % Output composite variable on client
c{:}    % Output composite variable on client
B       % Output distributed matrix on client
```

Distributed Matrix multiplication

- The distributed function can be used for parallel computing without using spmd.

```
A=randn(n); B=randn(n);
a=zeros(n); b=zeros(n); c=zeros(n);

parpool(4)
a = distributed(A);      % Distributes A, B. a, b are distributed
b = distributed(B);
tic
c = a * b;       % Run the multiplication in parallel by workers. c is distributed.
toc
delete(gcp)
```

spmd (6): Codistributed matrices

- Use codistributed within spmd region

```
n=1000;  A = rand(n);  B = rand(n);    % create matrices A and B on client
spmd
   u = codistributed(A, codistributor1d(1));    % distribute A by row
   v = codistributed(B, codistributor1d(2));    % distribute B by column, so that A and B are codistributed.
   w = u * v;        % run in parallel by workers; the result w is distributed.
   p = rand(n, codistributor1d(1));    % create distributed matrix p on workers
   q = codistributed.rand(n);    % create distributed matrix q on workers; p and q are codistributed
   s = p * q;        % run in parallel by workers; the result s is distributed
end
x=3+w    % use w directly on client
y=2*s     % use s directly on client
```

Exercise 2

- Compute the value of Pi (using spmd)

i) Write a parallel code for computing the value of Pi using spmd .

ii) Compare the performances of the serial, the parfor parallel and the spmd parallel codes.

(Hints: Distribute the grid to workers and compute local sum on all workers, then use the function gplus to compute the total sum.)

A Solution to Exercise 2

```
n=5000000000;  dx=1/n;    total_sum=Composite();      % total_sum will be modified in and used out of spmd region
tic       % start measuring time
spmd    % start spmd region
    m=n/numlabs;           % number of grid points on each worker
    length=1/numlabs;    % grid length on each worker
    startx = (labindex -1)*length;   % starting  x of the current worker
    endx = labindex*length;           % ending  x of the current worker
    x = startx : dx : endx;    % the portion of x held by the current worker
    local_sum=0;        % set 0 before accumulating
    local_sum = sum( 4. / (1. + x .* x) );     % compute local sum on the current lab
    total_sum = gplus(local_sum, 1);      % add up all local sums and store it on lab 1
end     % end spmd region
toc      % end measuring time
format long
pi=total_sum{1}*dx    % get the value of total_sum from worker 1 and output the result on client
```

Using Matlab on GPU (1)

- For many problems, GPUs achieve better performance than CPUs.
- MATLAB GPU utilities are growing.

- Matrix operations on GPU:

```
n = 6400;           % matrix size, better to be multiple of GPU warp-size (i.e. 32).
a = rand(n);        % cerate n * n random matrix a on base workspace (host)
A = gpuArray(a);        % A is created on GPU. The value of a is copied to A.
B = gpuArray.rand(n);   % Create random matrix directly on GPU
C = A * B;          % Matrix multiplication is computed on GPU
c = gather(C);      % bring result back to base workspace on CPU/host
```

Using Matlab on GPU (2)

- arrayfun: Apply function to each element of array on GPU.

```
n=10;
a = rand(n,1,'gpuArray');      % create random arrays on GPU
b = rand(n,1,'gpuArray');
c = rand(n,1,'gpuArray');
R = arrayfun( @(x,y,z)(x.*y+z), a, b, c );      % compute arrayfun on GPU
results = gather(R)     % bring result back to base workspace on CPU/host
```

Further Information

- MathWorks Web:
- ✓ MATLAB Parallel Computing Toolbox documentation: http://www.mathworks.com/help/distcomp/index.html

- BU Research Computing Services (RCS) Web:
- ✓ MATLAB Parallel Computing Toolbox:

http://www.bu.edu/tech/support/research/software-and-programming/common-languages/matlab/pct/

- A book: *Accelerating MATLAB Performance: 1001 tips to speed up MATLAB programs* by *Yair M. Altman*

- RCS help: help@scc.bu.edu , shaohao@bu.edu