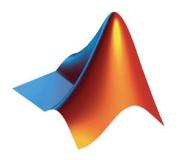


WORKSHOP: Parallel Computing With MATLAB (Part I)

Raymond Norris
Application Engineer
November 2023

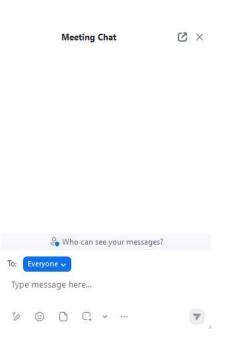






Meeting Chat

Please send chats to Everyone





Agenda

- Part I Parallel Computing with MATLAB on the Desktop
 - Parallel Computing Toolbox
 - MATLAB Online
- Part II Scaling MATLAB to Karolina
 - MATLAB Parallel Server
 - Karolina OnDemand





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- Part I Parallel Computing with MATLAB on the Desktop
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Why use parallel computing?



Save time with parallel computing by carrying out computationally and data-intensive problems in parallel (simultaneously)

- distribute your tasks to be executed in parallel
- distribute your data to solve big data problems on your compute cores and GPUs or scaled up to clusters and cloud computing



Why use parallel computing with MATLAB?

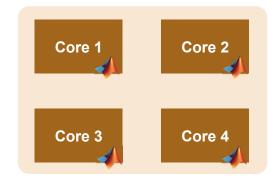


Save time with parallel computing by carrying out computationally and data-intensive problems in parallel (simultaneously)

- distribute your tasks to be executed in parallel
- distribute your data to solve big data problems

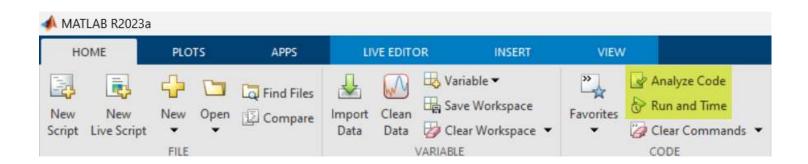
on your compute cores and GPUs or scaled up to clusters and cloud computing with minimal code changes, so you can focus on

your research



CPU with 4 cores





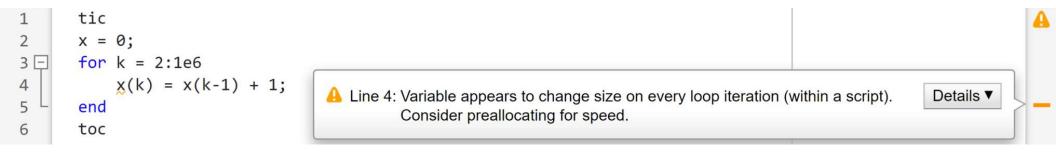


 Use the Profiler to find the code that runs slowest and determine possible performance improvements

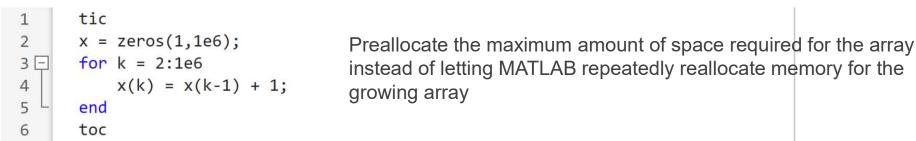
```
rng(1)
x = rand(1,1e6);
for k = 1:numel(x)
    if x(k) < .5
        x(k) = 0;
                                                         Use vectorization (matrix and vector operations)
    end
                                                         instead of for-loops
end
                Calls
                         Line
        Time
         0.035
                      1
                                rna(1)
         0.012
                               x = rand(1.1e6);
                                                              Time
                                                                      Calls
                                                                               Line
        < 0.001
                      1
                                for k = 1:numel(x)
                                                                                      rng(1)
                                                               0.007
                                                                            1
         0.061 1000000
                                    if x(k) < .5
                                                               0.011
                                                                                      x = rand(1.1e6)
         0.026
                499837
                                        x(k) = 0:
                                                               0.007
                                                                                      x(x<.5) = 0;
         0.048 1000000
                                    end
                                end
         0.049 1000000
```



 Use the Code Analyzer to automatically check your code for coding (and performance) problems



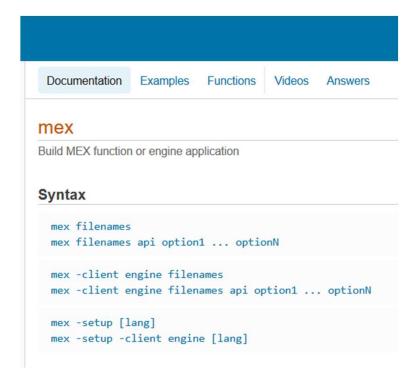
Elapsed time is 0.075824 seconds.



Elapsed time is 0.013109 seconds.



Replace code with MEX functions



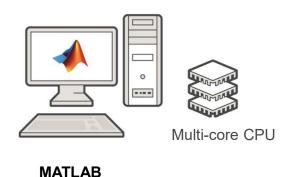


Before going parallel, optimize your code for the best performance with efficient programming practices

- Pre-allocate memory instead of letting arrays be resized dynamically
- → **Vectorize** Use matrix and vector operations instead of for-loops
- Try using functions instead of scripts. Functions are generally faster
- Create a new variable rather than assigning data of a different type to an existing variable
- Place independent operations outside loops to avoid redundant computations
- Avoid printing too much data on the screen, reuse existing graphics handles



MATLAB has built-in multithreading







MATLAB Multicore

Q

Run MATLAB on multicore and multiprocessor machines

MATLAB® provides two main ways to take advantage of multicore and multiprocessor computers. By using the full computational power of your machine, you can run your MATLAB applications faster and more efficiently.

Built-in Multithreading

Linear algebra and numerical functions such as fft, \ (mldivide), eig, svd, and sort are multithreaded in MATLAB. Multithreaded computations have been on by default in MATLAB since Release 2008a. These functions automatically execute on multiple computational threads in a single MATLAB session, allowing them to execute faster on multicore-enabled machines. Additionally, many functions in Image Processing ToolboxTM are multithreaded.

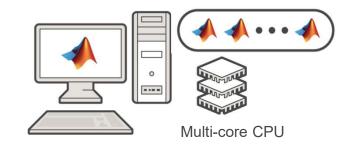
Parallelism Using MATLAB Workers

You can run multiple MATLAB workers (MATLAB computational engines) on a single machine to execute applications in parallel, with Parallel Computing Toolbox™. This approach allows you more control over the parallelism than with built-in multithreading, and is often used for coarser grained problems such as running parameter sweeps in parallel.

MATLAB multicore 13



Scale further with parallel computing



MATLAB
Parallel Computing Toolbox



Run MATLAB on multicore and multiprocessor machines

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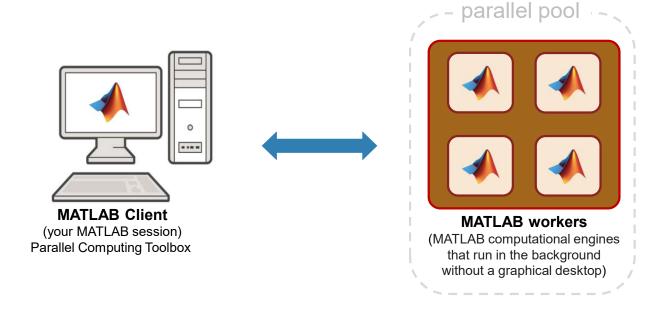
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MATLAB multicore 15



Run parallel code by utilizing multiple CPU cores





Download Instructions

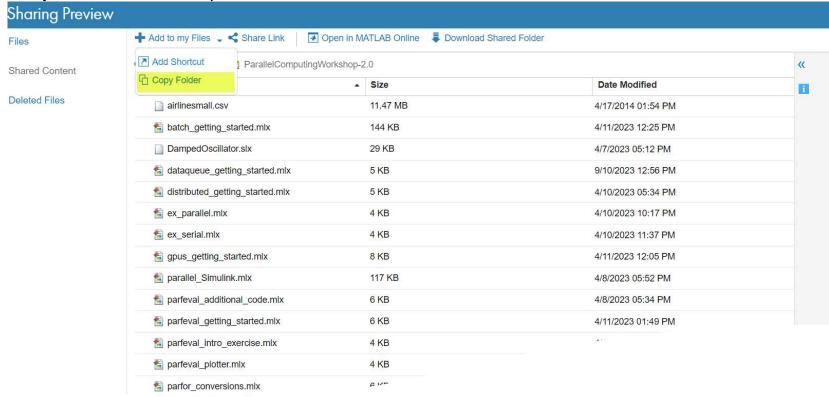
- https://tinyurl.com/ParallelComputingWorkshop
 - Click on Add to my Files
 - Click Copy Folder
- https://www.mathworks.com/licensecenter/classroom/4234856
- Click Access MATLAB Online (maybe prompted to sign-in again)
 - Click Open MATLAB Online
 - In Current Folder, double click on ParallelComputingWorkshop-2.0



Setup: Step 1 – Copy materials via MATLAB Drive

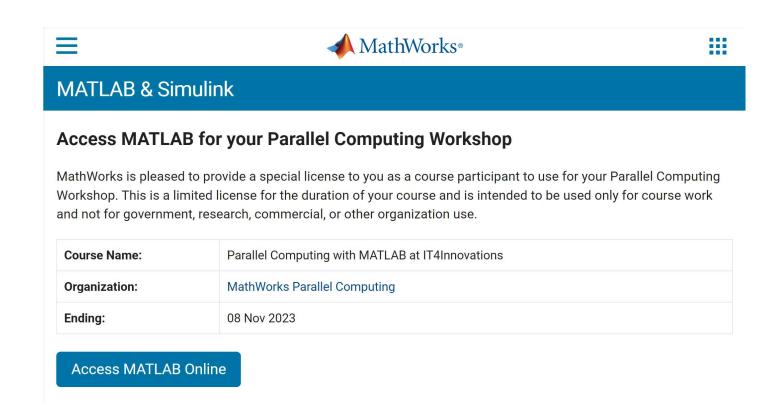
Click Add to my Files and then click Copy Folder.

For use on your MATLAB Desktop, click **Download Shared Folder** instead.





Setup: Step 2 – Launch MATLAB Online





Hands-On Exercise: Starting a parallel pool

parpool Introduction

The purpose of this excercise is to learn what is a parallel pool and the different ways to start and shut it down.

To get started, run the following command:

doc parpool

Start a parallel pool programmatically

Start an interactive parallel pool of 2 workers through the command line.

% TODO: Start an interactive parallel pool of 2 workers programatically

What happens if you try to run the above command a second time?

% TODO: Rerun the section to start another pool

Only one interactive parallel pool can be open at a time.



Scaling MATLAB applications and Simulink simulations

Ease of Use

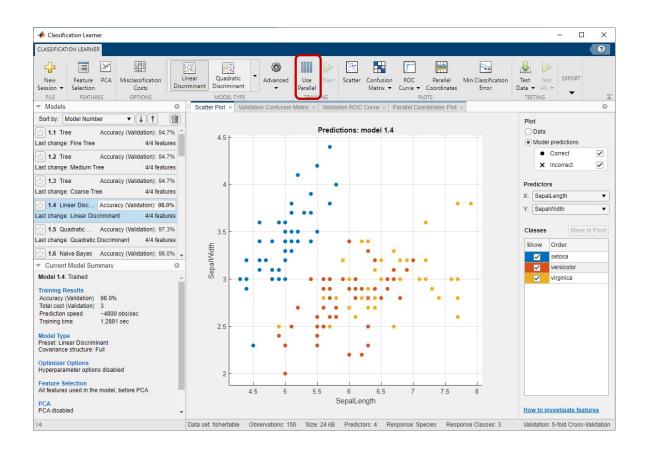
Automatic parallel support in toolboxes

Common programming constructs

Advanced programming constructs



Automatic parallel support in toolboxes



Scaling MATLAB applications and Simulink simulations



Ease of Use

Automatic parallel support in toolboxes

Common programming constructs

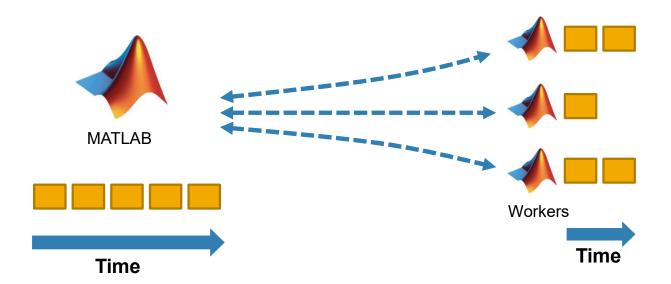
(parfor, parfeval, parsim, ...)

Advanced programming constructs



Explicit parallelism using parfor (parallel for-loop)

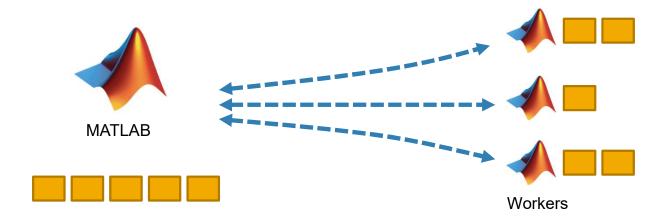
- Run iterations in parallel
- Examples: parameter sweeps, Monte Carlo simulations





Explicit parallelism using parfor

```
a = zeros(5, 1);
b = pi;
for i = 1:5
    a(i) = i + b;
end
disp(a)
a = zeros(5, 1);
b = pi;
parfor i = 1:5
    a(i) = i + b;
end
disp(a)
```





Hands-On Exercise: Writing our first parfor

Getting Started with parfor

In this exercise, we will rewrite a simple for-loop into a parfor-loop and understand the basic differences between the two types of loops.

```
doc parfor
```

How much time will the following for-loop take?

This is an example of a basic for-loop; in each iteration, pause(1) stops MATLAB execution for one second and then displays the index idx of the iteration. Since there are 10 iterations, the for-loop takes about 10 seconds (the added tic and toc measure the time elapsed) and the indices are displayed sequentially, from 1 to 10.

```
tic
for idx = 1:10
    pause(1)
    disp(idx)
end
toc
```



DataQueue: Execute code as parfor iterations complete

 Send data or messages from parallel workers back to the MATLAB client

 Retrieve intermediate values and track computation progress

```
function a = parforWaitbar
D = parallel.pool.DataQueue;
h = waitbar(0, 'Please wait ...');
afterEach(D, @nUpdateWaitbar)
N = 200;
p = 1;
parfor i = 1:N
    a(i) = max(abs(eig(rand(400))));
    send(D, i)
end
    function nUpdateWaitbar(~)
      waitbar(p/N, h)
        p = p + 1;
    end
end
                       Please wait ...
```



Hands-On Exercise: Sending data with a dataqueue

Getting Started with dataqueue

In this exercise, we will use a parallel data queue to send data from the workers to the MATLAB client.

doc dataqueue

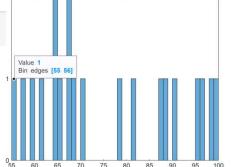
Give the quiz

In this problem, we are giving a quiz to 20 students. Each student will finish in a random period of time (max 5 minutes) and each student will get a random grade between 55 and 100.

We need to gather all of the scores to plot the results, but we also want to write the results as they happen in real-time to a "database" (the MATLAB Command Window in this case).

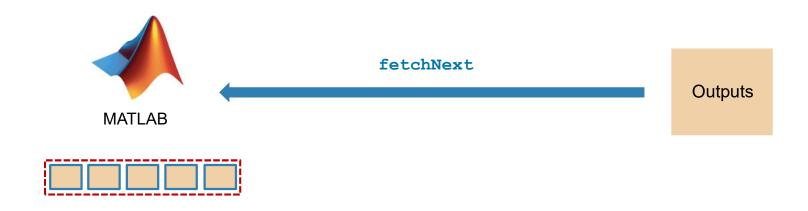
The for-loop will gather all the scores to eventually be plotted in a histogram, but MATLAB should also be listening to "events" (when the grade get posted) in the dataqueue.

```
% Create a data queue so workers can send the grade back to the client once
% their done
%
TODO: Create a dataqueue object, q.
```





Execute functions in parallel asynchronously using parfeval



Asynchronous execution on parallel workers Useful for "needle in a haystack" problems

```
for idx = 1:10
    f(idx) = parfeval(@magic,1,idx);
end

for idx = 1:10
    [completedIdx,value] = fetchNext(f);
    magicResults{completedIdx} = value;
end
```



Run code in parallel

Synchronously with parfor

- You wait for your loop to complete to obtain your results
- Your MATLAB client is blocked from running any new computations
- You cannot break out of loop early

Asynchronously with parfeval*

- You can obtain intermediate results
- Your MATLAB client is free to run other computations
- You can break out of loop early



Hands-On Exercise: Use parfeval to run functions in the background

parfeval Plotter

Parallelize the code so that plots are done as quickly as possible. How do we get the plot to show the results? How can we view and plot intermediate results as the computation progresses?

Hint: Try parfor and parfeval

```
figure('Name','for')
hold on

tic
for idx = 1:100
    y = calc(idx);
    plot(idx,y,'o')
end
toc
```

parfor plotter solution 1

This solution demonstrates how to use a parfor-loop to speed



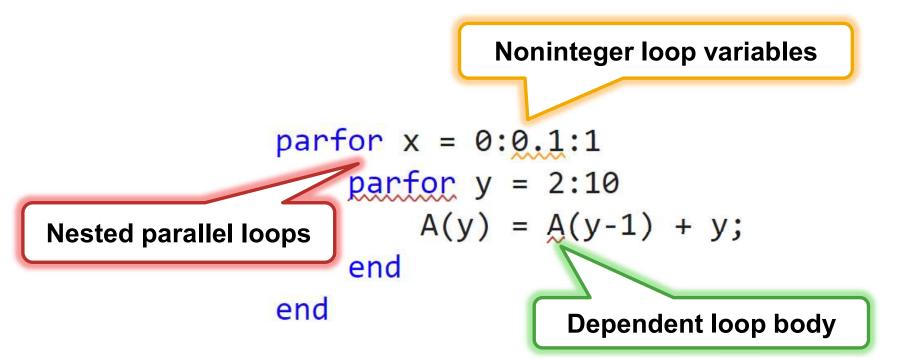
Use Code Analyzer to fix problems when converting for-loops to parfor-loops

parfor-loop iterations have no guaranteed order, and one loop iteration cannot depend on a previous iteration; therefore, you may need to rewrite your code to use parfor

```
a = zeros(5, 1);
                                                                                                                      No warnings found.
       b = pi;
                                                                                                                      (Using Default Settings)
      Eparfor i = 1:5
3
             a(i) = i + b;
5
       end
        disp(a)
        a = zeros(5, 1);
        b = pi;
3
      Eparfor i = 2:6
              a(i) = a(i-1) + b;
4
                                                         Line 4: In a PARFOR loop, variable 'a' is indexed in different ways, potentially causing dependencies between iterations.
5
        end
        disp(a)
```



Common problems when rewriting a for-loop as a parfor-loop





Hands-On Exercise: Rewrite for-loops into parfor-loops

Rewriting for-Loops As parfor-Loops

This example focus on diagnosing and fixing issues you may run into rewriting a for-loop to a parfor-loop.

Hint: Review the code analyzer messages and check the documentation for additional help.

Ensure parfor-loop iterations are task independent

When you rewrite for-loops to parfor-loops, you need ensure that your parfor-loop iterations are independent. parfor-loop iterations have *no guaranteed order*, while the iteration order in for-loops is *sequential*.

Review the code below which was rewritten as a parfor-loop and the code analyzer messages - is this code suitable for parallelization?

```
len = 10;
A = [0 nan(1,len-1)];
parfor idx = 2:len
    A(idx) = A(idx-1) + rand;
end
```

the narfor loop variable is



Hands-On Exercise: Refactoring for-loops

Loading and Saving in parfor

One way to avoid issues that arise from rewriting for-loops to parfor-loops is to refactor the loop. The following example illustrates a best practice when rewriting loops.

Rewrite the for-loop as a parfor-loop.

```
for idx = 1:4
    load xy.mat
    z = x*y*rand;
    save(['z' num2str(idx) '.mat'], 'z')
end
```

First attempt

parfor-loops need to be able to classify each variable inside their block. View the parfor transparency documentation for help getting started. Once a variable has been classified, it can not change its classification. In the above countries that x and y are variables (they are assumed to be functions) introduces new variables when the parfor is running -- a violation of the countries of the co



Consider parallel overhead* in deciding when to use parfor

parfor can be useful ©

- for-loops with loop iterations that take long to execute
- **for**-loops with **many** loop iterations that take a short time, e.g., parameter sweep

parfor might not be useful \otimes

 for-loops with loop iterations that take a short time to execute

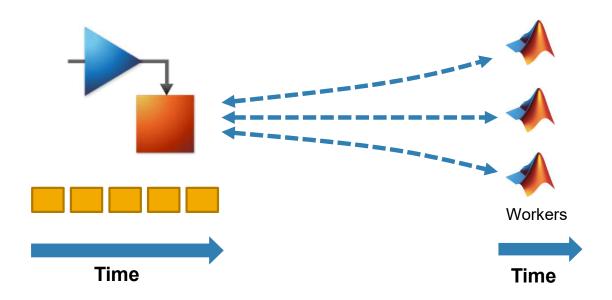
Ways to improve **parfor** performance:

- Experiment which is faster: creating arrays before the loop or have each worker create its own arrays inside the loop (saves transfer time, especially on a remote cluster)
- Use sliced variables or temporary variables
- ... Check <u>mathworks.com/help/parallel-computing/improve-parfor-performance.html</u>

^{*} Parallel overhead: time required for communication, coordination, and data transfer from client to workers and back



Run multiple simulations in parallel with parsim



 Run independent Simulink simulations in parallel using the parsim function

```
for i = 10000:-1:1
    in(i) = Simulink.SimulationInput(my_model);
    in(i) = in(i).setVariable(my_var, i);
end
out = parsim(in);
```



Hands-On Exercise: Parameters sweeps with Simulink

Parallel Simulation with parsim

In this exercise, we'll run a parallel sweep through a Simulink model.

```
doc Simulink.SimulationInput
doc parsim
doc batchsim
```

Damping and stiffness

We are going to run a parameter sweep over different combinations of damping and stiffness. Define a grid of all combinations.

```
bNum = 5;
kNum = 5;
bVals = linspace(0.1, 5, bNum); % damping
kVals = linspace(1.5, 5, kNum); % stiffness
[kGrid, bGrid] = meshgrid(bVals, kVals);
```



Scaling MATLAB applications and Simulink simulations



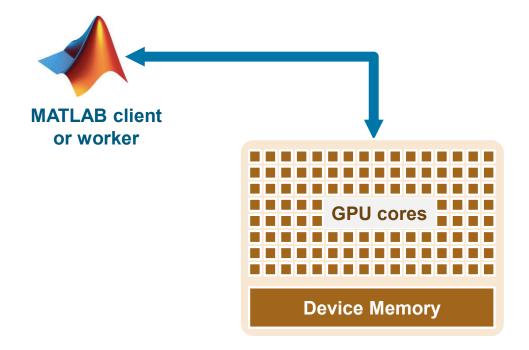
Automatic parallel support in toolboxes

Common programming constructs

Advanced programming constructs (spmd, etc.)



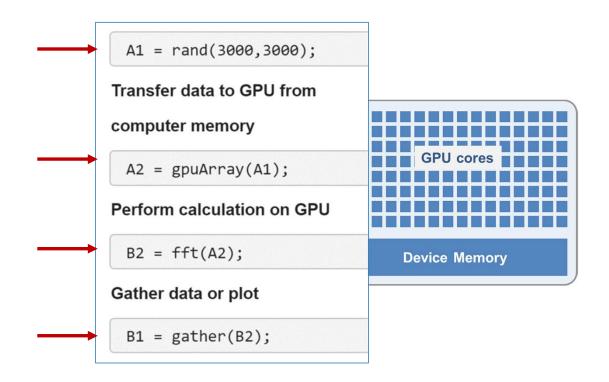
Leverage NVIDIA GPUs without learning CUDA





Leverage your GPU to accelerate your MATLAB code

- Ideal Problems
 - massively parallel and/or vectorized operations
 - computationally intensive
- 1000+ GPU-supported functions
- Use gpuArray and gather to transfer data between CPU and GPU



MATLAB GPU Computing



Hands-On Exercise: Offload computations to your GPU

Getting started with GPU Computing in MATLAB

This exercise will demonstrate how to speed up computations using your computer's GPU.

We'll start with an algorithm initially written to run on the CPU. If all the functions that you want to use are supported on the GPU, you can simply use gpuArray to transfer input data to the GPU and call gather to retrieve the output data from the GPU. With some minor changes to the code, we'll be able to offload the computation to the GPU.

Run a computation on the CPU

Compute the fft of a random matrix.

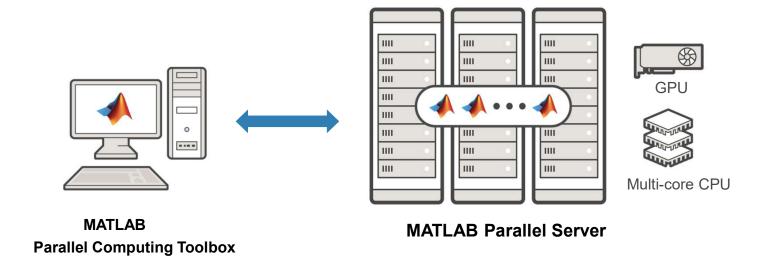
```
N = 8192;
matrix_cpu = rand(N,N);

tic
out_cpu = fft(matrix_cpu);
time_cpu = toc;

disp(['FFT time on CPU: ' num2str(time_cpu)])
```



Parallel computing on your desktop, clusters, and clouds



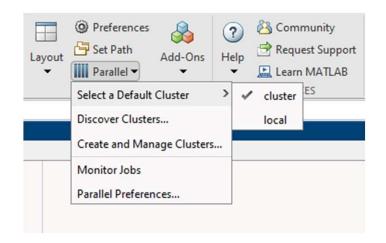
- Prototype on the desktop
- Integrate with infrastructure
- Access directly through MATLAB



Scale to clusters and clouds

With MATLAB Parallel Server, you can...

- Change hardware with minimal code change
- Submit to on-premise or cloud clusters
- Support cross-platform submission
 - Windows client to Linux cluster

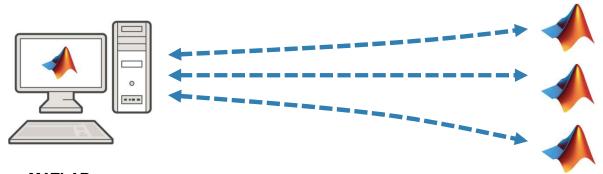




Interactive parallel computing

Leverage cluster resources in MATLAB

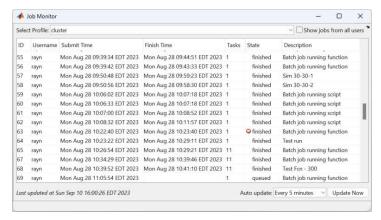
- >> parpool('cluster', 3);
- >> myscript



MATLAB Parallel Computing Toolbox

myscript.m

```
a = zeros(5, 1);
b = pi;
parfor i = 1:5
   a(i) = i + b;
end
```





Run a parallel pool from specified profile

On local machine

- Start parallel pool of local workers parpool ('Processes');
- Start parallel pool of thread workers

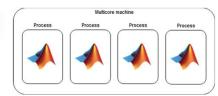
```
parpool('Threads');
```

- © Reduced memory usage, faster scheduling, lower data transfer costs
- Thread-based environments support only a subset of the functions available for process workers

On cluster

 Start parallel pool using cluster object

```
c = parcluster;
parpool(c);
```

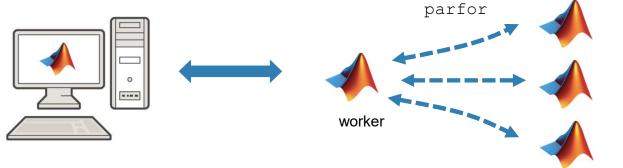




batch simplifies offloading computations

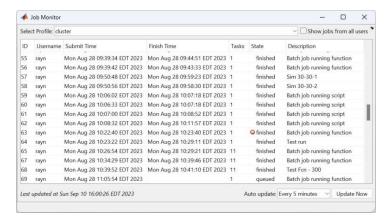
Submit MATLAB jobs to the cluster





MATLAB Parallel Computing Toolbox







Hands-On Exercise: Use batch to offload serial and parallel computations

Getting Started with batch

You can use batch jobs to offload the execution of long-running computations in the background and carry out other tasks while the batch job is processing. batch does not block MATLAB; allowing you to continue working while computations take place in the background. When you submit batch jobs to another computer or cluster, you can close MATLAB on the client and retrieve results later.

In this exercise, you will submit batch jobs from MATLAB to your local machine. The workers will run on the same machine as the client, but the same workflow can be used to submit jobs to a remote compute cluster or the cloud, freeing up your local resources.

Note: Close parallel pool if it's open.

Run a batch job to offload serial computation

ex_serial performs, serially, N trials of computing the largest eigenvalue for an M-by-M random matrix. ex_serial is called as such

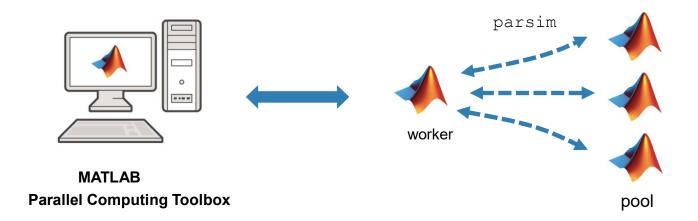
```
% matrix size: 50
% trials: 10000
1+ = ex serial(50,10000);
```



batch simplifies offloading simulations

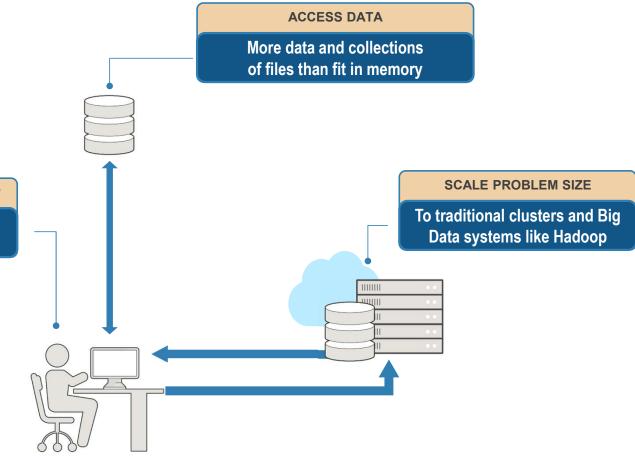
Submit Simulink jobs to the cluster

job = batchsim(in, 'Pool', 3);





Big Data Workflows



Adapt traditional processing tools or learn new tools to work with Big Data



tall arrays

- Data type designed for data that doesn't fit into memory
- Lots of observations (hence "tall")
- Looks like a normal MATLAB array
 - Supports numeric types, tables, datetimes, strings, etc.
 - Supports several hundred functions for basic math, stats, indexing, etc.
 - Statistics and Machine Learning Toolbox support (clustering, classification, etc.)





Hands-On Exercise: Use tall arrays for Big Data

Getting Started with tall arrays for Big Data

In this exercise we'll use tall arrays to work with large data sets that have more rows than might fit into memory.

You can work with many operations and functions as you would with in-memory MATLAB arrays, but most results are evaluated only when you request them explicitly using gather, write a tall array to disk, or visualize the tall array. MATLAB automatically optimizes the queued calculations by minimizing the number of passes through the data.

Access Data: Create Datastore from Sample File(s)

The comma-separated text file airlinesmall.csv contains departure and arrival information about individual airline flights from the years 1987 through 2008, stored in a tabular manner.

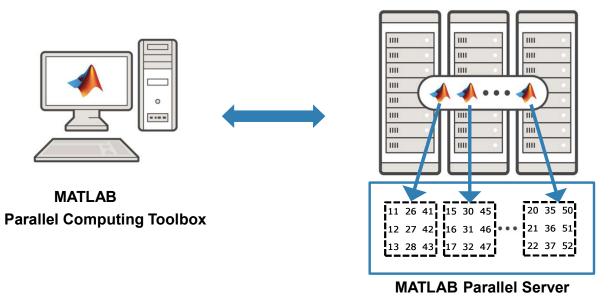
Tabular data that contains a mix of numeric and text data, as well as variable and row names, is best represented in MATLAB as a **table** (a container that stores column-oriented data in variables), because table variables can have different data types and sizes as long as all variables have the same number of rows.

If a file can be imported and processed in its entirety on our computer, we could also import the data in a table. either interactively, using the Import Tool, or programmatically, by reading the comma-separated function with at least the file name as an input parameter, and then apply



distributed arrays

- Distribute large matrices across workers running on a cluster
- Support includes matrix manipulation, linear algebra, and signal processing
- Several hundred MATLAB functions overloaded for distributed arrays



Working with distributed arrays



Hands-On Exercise: Use distributed arrays for Big Data

Getting Started with distributed arrays for Big Data

In this example, we will work with distributed arrays, to partition large arrays across workers. We operate on the entire array as a single entity, without having to worry about its distributed nature, as workers operate only on their part of the array, and automatically transfer data between themselves when necessary. Unlike tall arrays, distributed arrays are in the memory of your computer/cluster, but that memory is shared across multiple workers.

Create distributed arrays

You can create a distributed array in different ways.

For instance, you can use the distributed function to distribute an existing array from the client workspace to the workers of a parallel pool.

Let's open a parallel pool and create a 1000-by-1000 array of uniformly random numbers in the client workspace:

```
p = gcp;
a = rand(1000,1000);
```

Then let's use the distributed function to distribute the array to the works

```
1: -tributed(a).
```



tall arrays vs. distributed arrays

- tall arrays are useful for out-of-memory datasets with a "tall" shape
 - Can be used on a desktop, cluster, or with Spark/Hadoop
 - Low-level alternatives are MapReduce and MATLAB API for Spark
- distributed arrays are useful for in-memory datasets on a cluster
 - Can be any shape ("tall", "wide", or both)
 - Low-level alternative is SPMD + gop (Global operation across all workers)

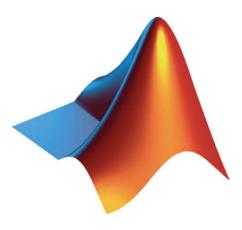
	Tall Array	Distributed Array
Support Focus	Data Analytics, Statistics and Machine Learning	Linear Algebra, Matrix Manipulations
Data Shape	"Tall" only	"Tall", "wide" or both
Prototype on Desktop	✓	✓
Helps on Desktop	✓	×
Run on HPC	✓	✓
Run on Spark/Hadoop	✓	×
Fault Tolerant	✓	×



Further Resources

- MATLAB Documentation
 - MATLAB → Software Development Tools → Performance and Memory
 - Parallel Computing Toolbox
- Parallel and GPU Computing Tutorials
 - https://www.mathworks.com/videos/series/parallel-and-gpu-computing-tutorials-97719.html
- Parallel Computing with MATLAB and Simulink
 - https://www.mathworks.com/solutions/parallel-computing.html





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