Workshop
Parallel Computing with MATLAB

Apr 30th 2024

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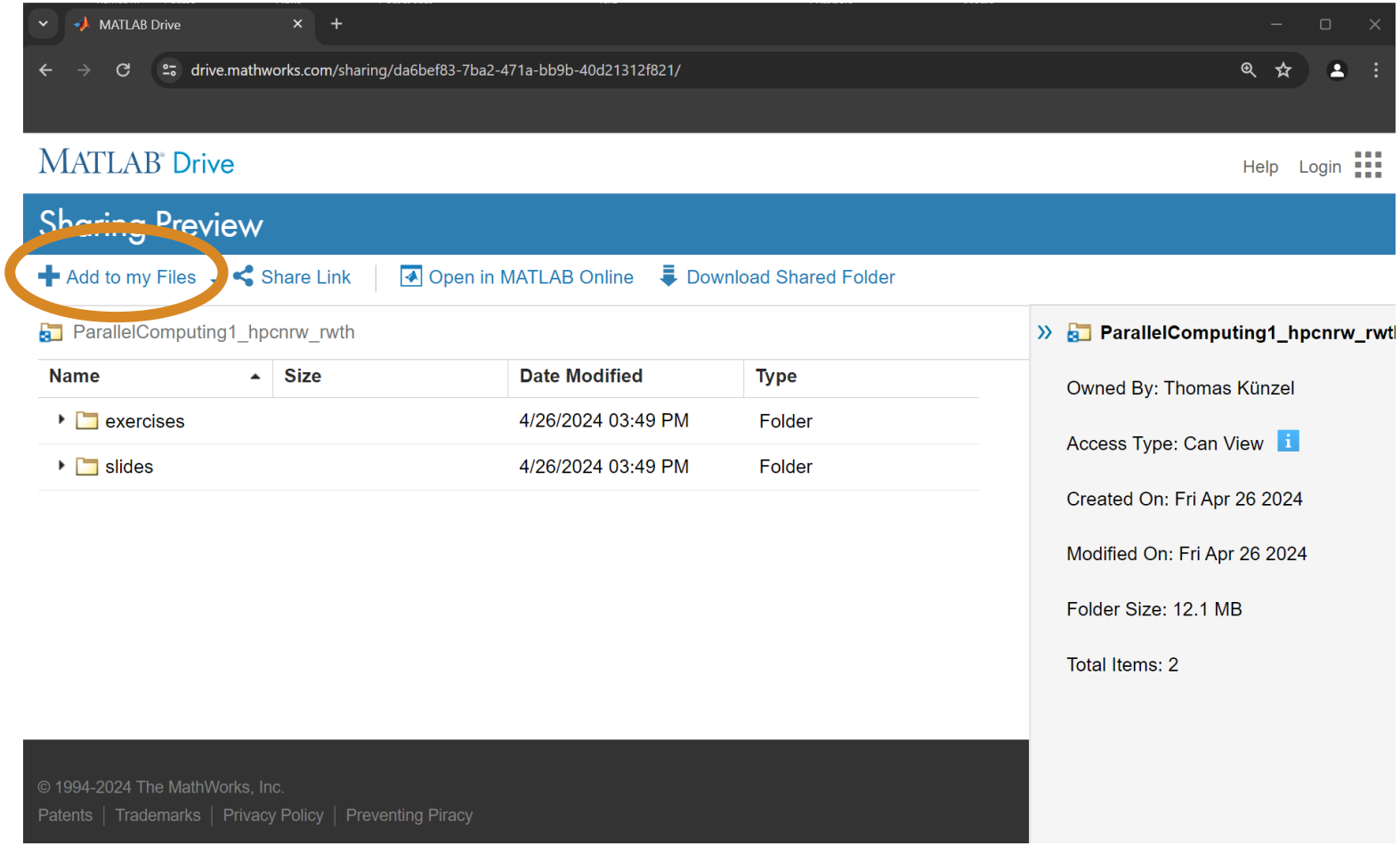
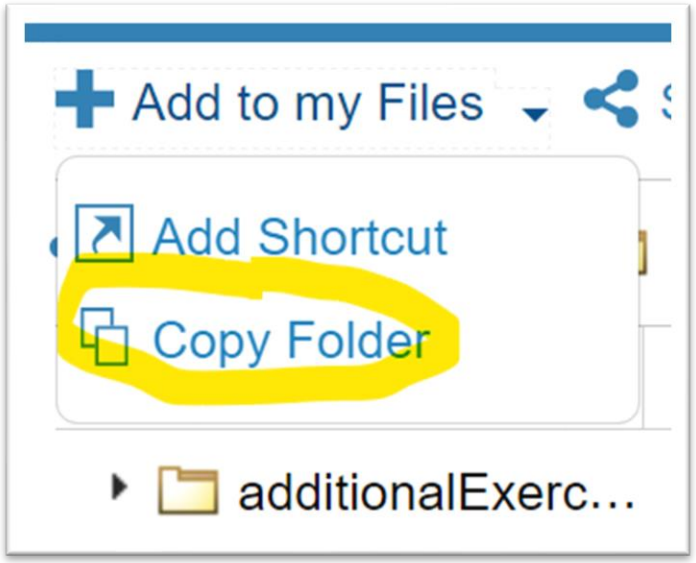
Agenda

- **Parallel Computing with MATLAB (Today)**
  - **Speeding up programs with parallel computing**
  - **GPU computing**
  - **Working with large data sets**
- ***Parallel Computing with MATLAB on the CLAIX Cluster (May 7th)***
- **Introduction to Research Software Development with MATLAB (May 14th)**
- **AI for Predictive Maintenance (May 21st)**

Setup: Step 1 – Copy materials via MATLAB Drive

Click **Add to my Files** and select **Copy Folder**.
*For use on your MATLAB Desktop, click **Download Shared Folder** instead.*





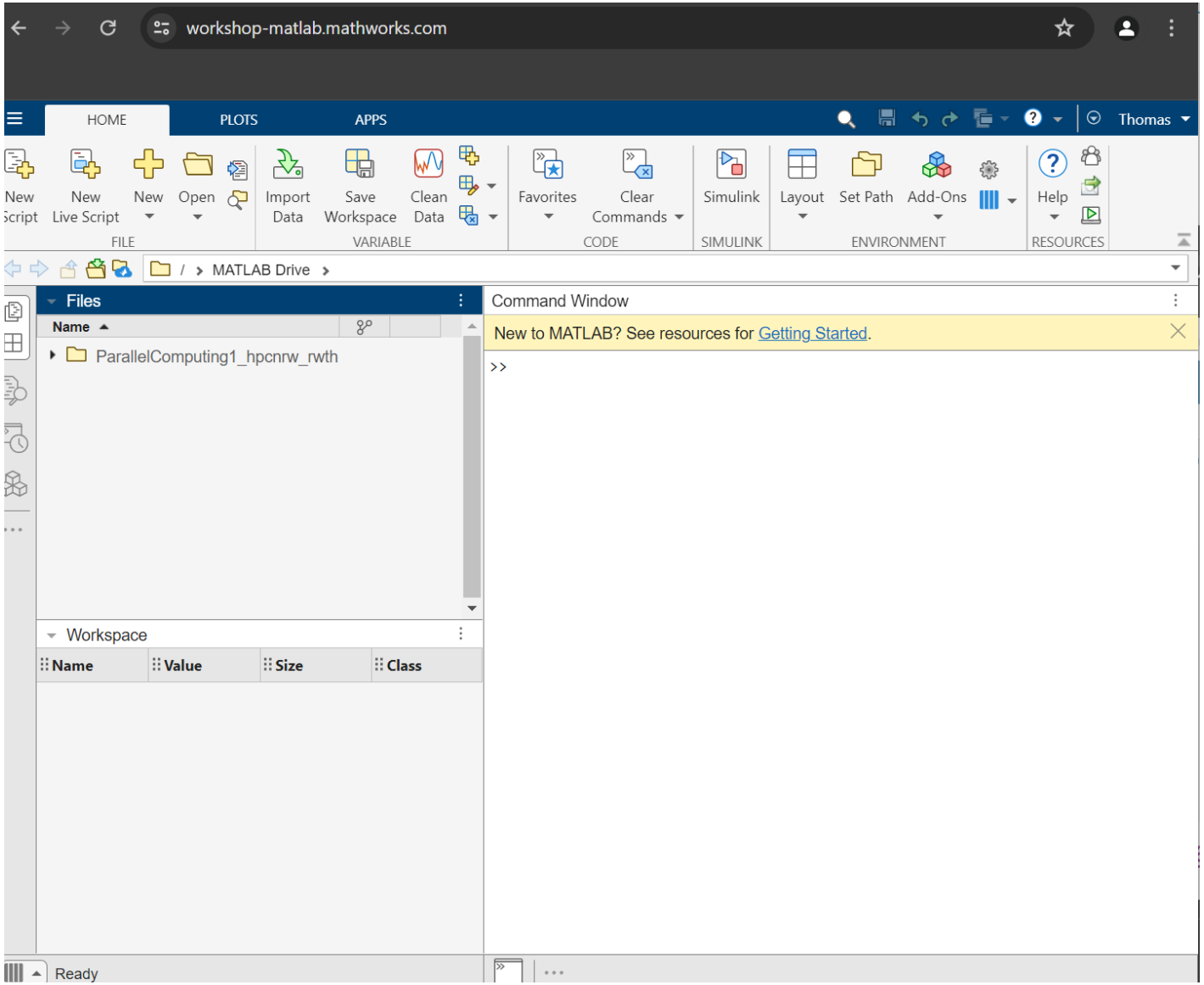
https://drive.mathworks.com/sharing/da6bef83-7ba2-471a-bb9b-40d21312f821

Setup: Step 2 – Activate the workshop license and launch MATLAB Online

Sign in to your MathWorks Account
→ Trial License will get associated temporarily

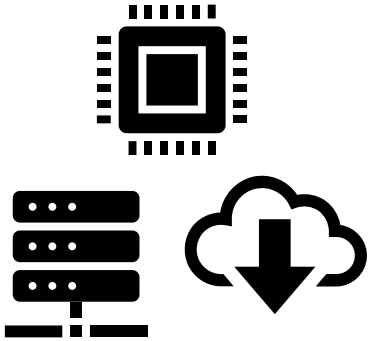
https://de.mathworks.com/licensecenter/classroom/4421700

Setup: Course Materials should be automatically added in your MATLAB Online



Why use parallel computing?

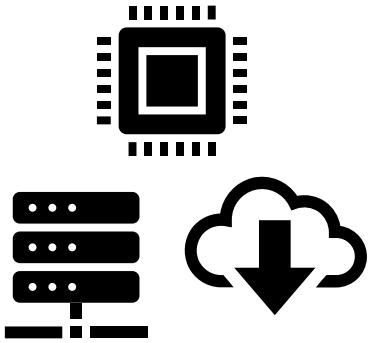
Solve your problem in a shorter time or tackle larger problems in the same amount of time.



Leverage multiple CPU or GPU cores available in one computer or employ the resources of multiple computers simultaneously by scaling to clusters and clouds!

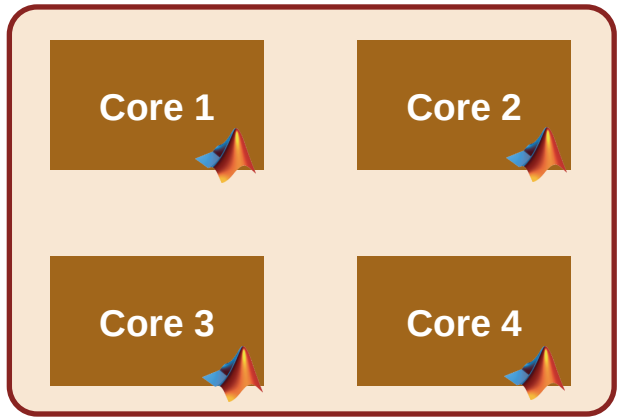
Why use parallel computing with MATLAB?

Solve your problem in a shorter time or tackle larger problems in the same amount of time.



Leverage multiple CPU or GPU cores available in one computer or employ the resources of multiple computers simultaneously by scaling to clusters and clouds!

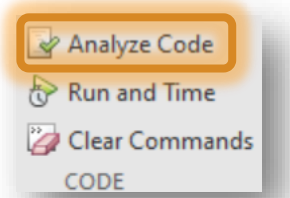
Do this with minimal code changes, so you can focus on your research use case.



CPU with 4 cores

! Before going parallel, make sure you optimize your serial code for best performance

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




```
1  tic
2  x = 0;
3  for k = 2:1e6
4      x(k) = x(k-1)+1;
5  end
6  toc
```

Elapsed time is 0.091058 seconds.

⚠ Line 4: Variable appears to change size on every loop iteration (within a script). Consider preallocating for speed. Details ▾

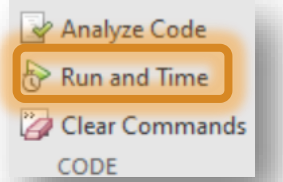
```
1  tic
2  x = zeros(1,1e6);
3  for k = 2:1e6
4      x(k) = x(k-1)+1;
5  end
6  toc
```

Elapsed time is 0.018484 seconds.

! Preallocating the maximum amount of space required for the array instead of letting MATLAB repeatedly reallocate memory for the growing array is about 5 times faster!

! Before going parallel, make sure you optimize your serial code for best performance

- Use the **Profiler** to find the code that runs slowest and evaluate possible performance improvements.




```
1  rng(1)
2  x = rand(1,1e6);
3  for k = 1:numel(x)
4      if x(k)<.5
5          x(k) = 0;
6      end
7  end
8
```

! Use vectorization (matrix and vector operations) instead of for-loops!

Time	Calls	Line	
0.008	1	1	rng(1)
0.010	1	2	x = rand(1,1e6);
< 0.001	1	3	for k = 1:numel(x)
0.041	1000000	4	if x(k)<.5
0.016	499837	5	x(k) = 0;
0.032	1000000	6	end
0.032	1000000	7	end

Time	Calls	Line	
0.005	1	1	rng(1)
0.010	1	2	x = rand(1,1e6);
0.007	1	3	x(x<.5) = 0;

! Before going parallel, make sure you optimize your serial code for best performance with efficient programming practices

- **Pre-allocate memory** instead of letting arrays be resized dynamically
- **Prefer shipped code** over custom written code for the same functionality.
- **Write functions** – functions are optimized by the just-in-time compiler and are cleaner code.
- 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 text to the output; reuse existing graphics handles.

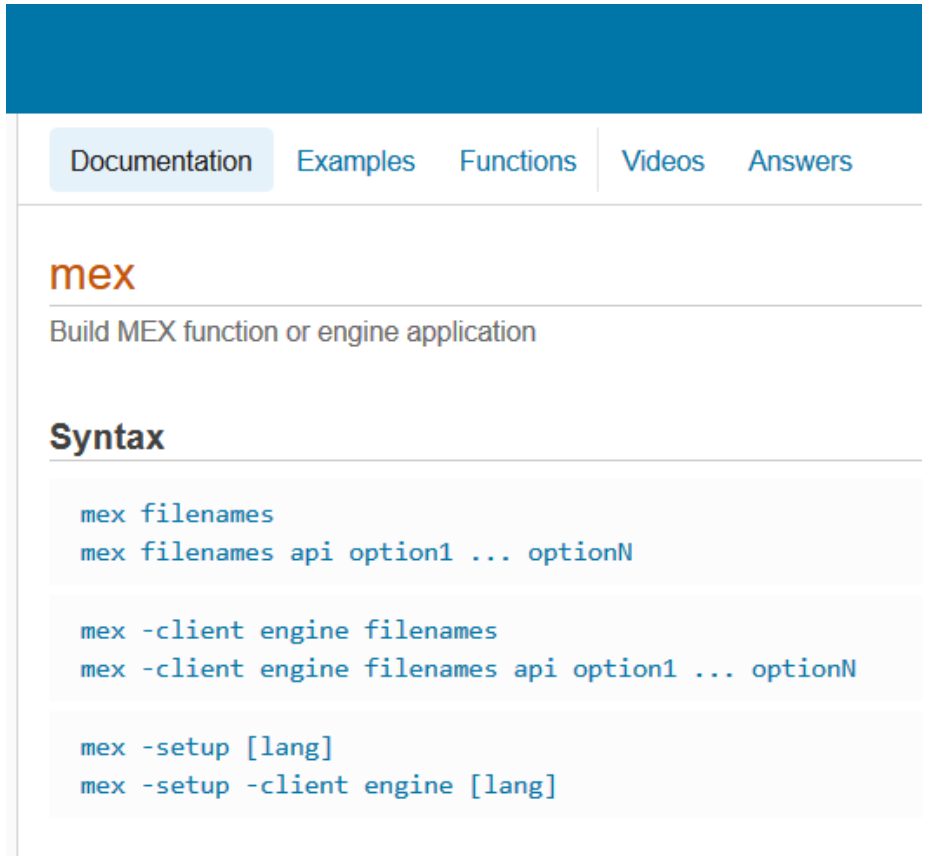
Techniques to improve performance

What about "**Vectorization**"? Weren't for-loops slow? This is not true any more in modern MATLAB!

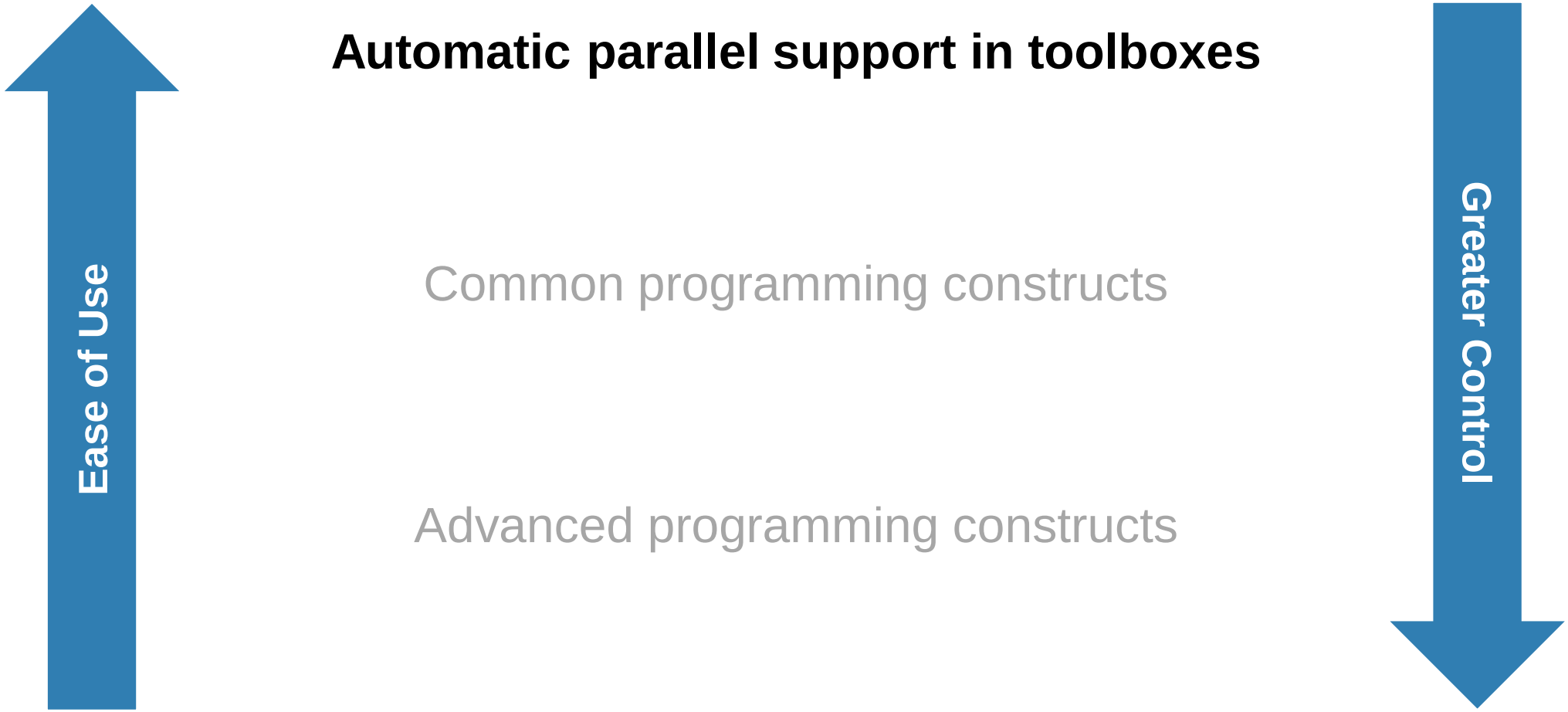
Write the code as you think about the problem!

! Before going parallel, make sure you optimize your serial code for best performance with efficient programming practices

(Advanced) Replace code with MEX functions



Scaling MATLAB applications and Simulink simulations



Take advantage of your multicore and multiprocessor computers automatically

with no programming effort
using built-in multithreading

just by setting a flag/preference
* with Parallel Computing Toolbox

MATLAB Multicore

What Is MATLAB Multicore?

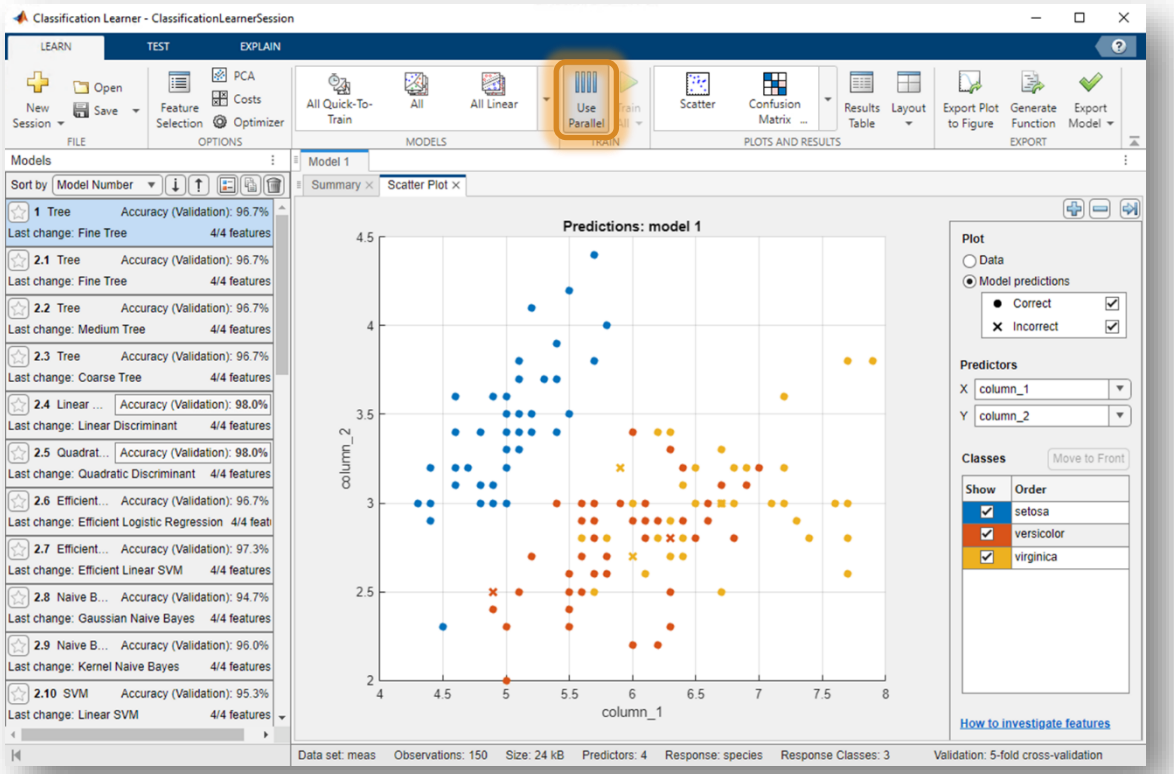
MATLAB® provides two main ways to take advantage of multicore and multiprocessor computers. By using the full computational power of your machine, you can run your MATLAB applications faster and more efficiently.

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 Toolbox™ 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.



Scaling MATLAB applications and Simulink simulations

Automatic parallel support in toolboxes

Common programming constructs
(`parfor, parfeval, parsim, …`)

Advanced programming constructs

Scale further with parallel computing

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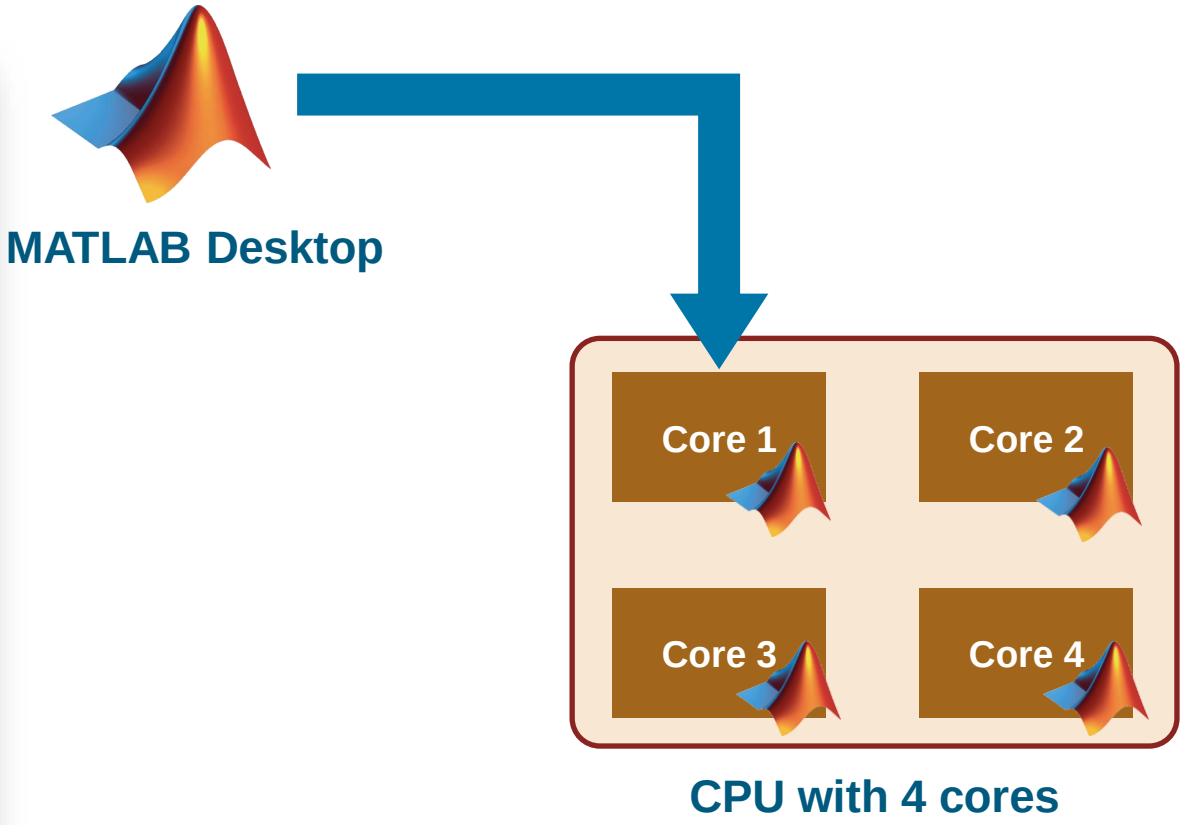
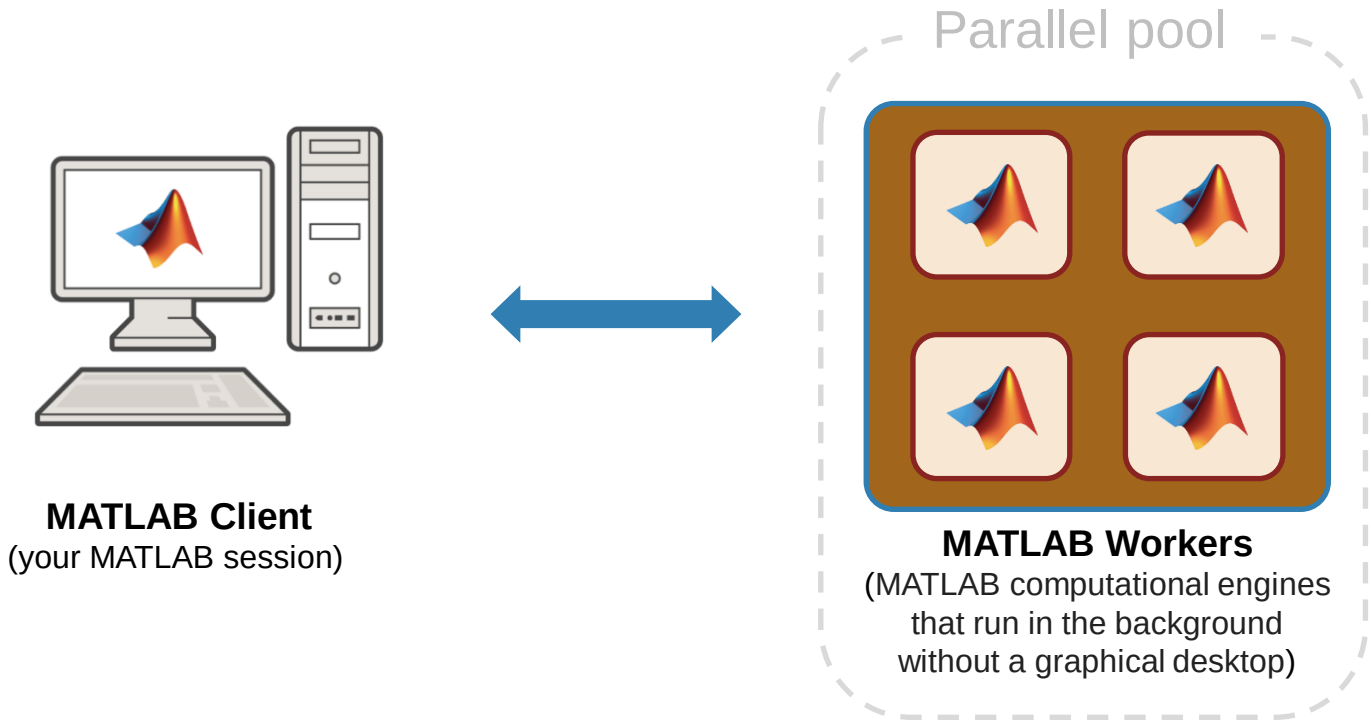
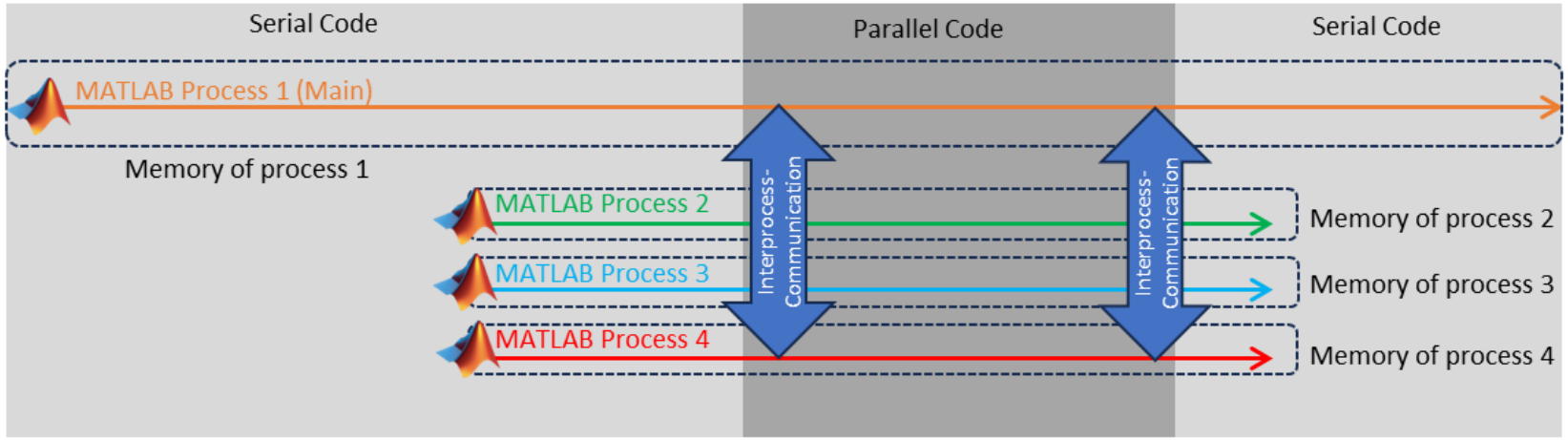


Run multiple iterations by utilizing multiple CPU cores

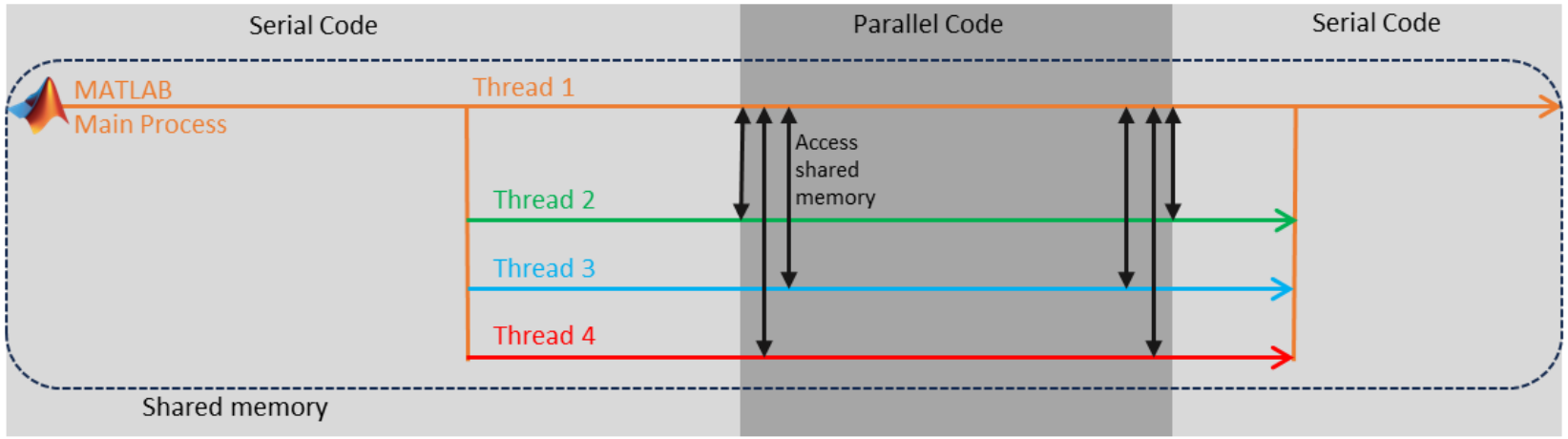


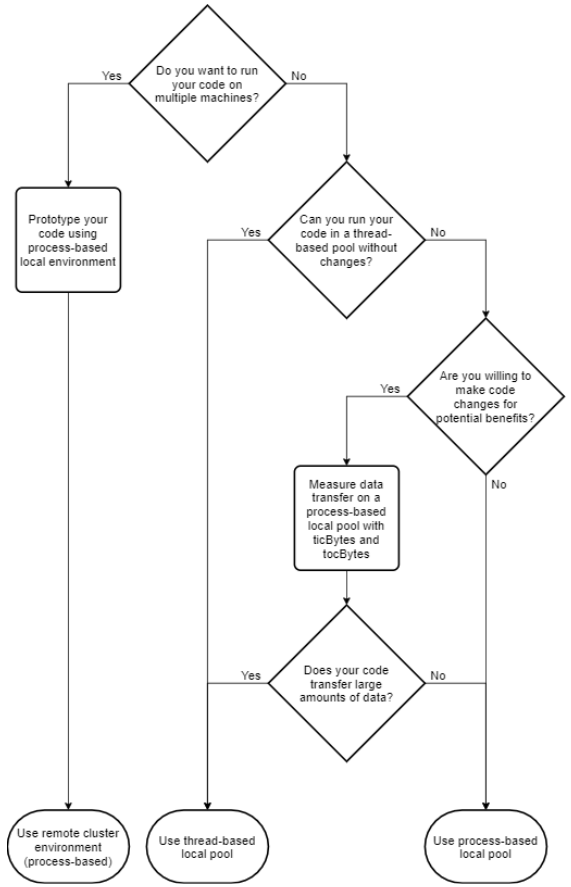
Parallel Pool as Processes vs. Threads

"Processes"



"Threads"

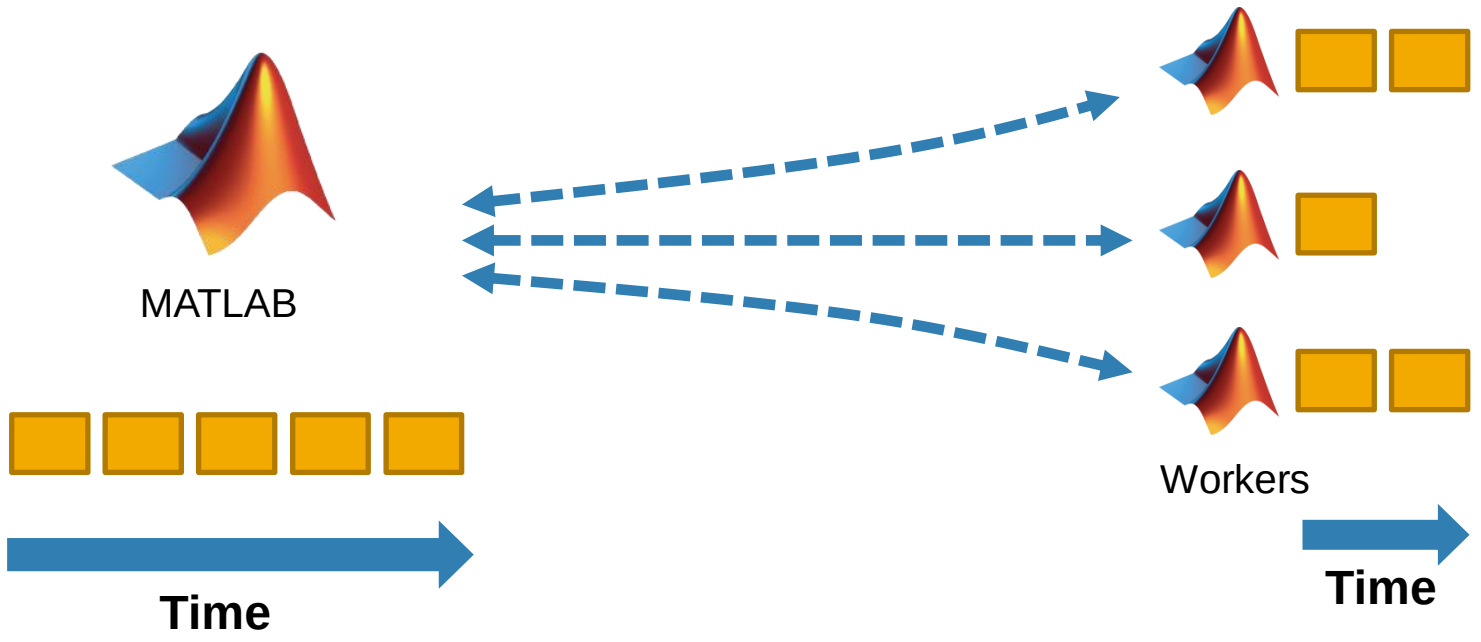




[Choose Between Thread-Based and Process-Based Environments - MATLAB & Simulink (mathworks.com)]

Explicit parallelism using `parfor` (parallel `for`-loop)

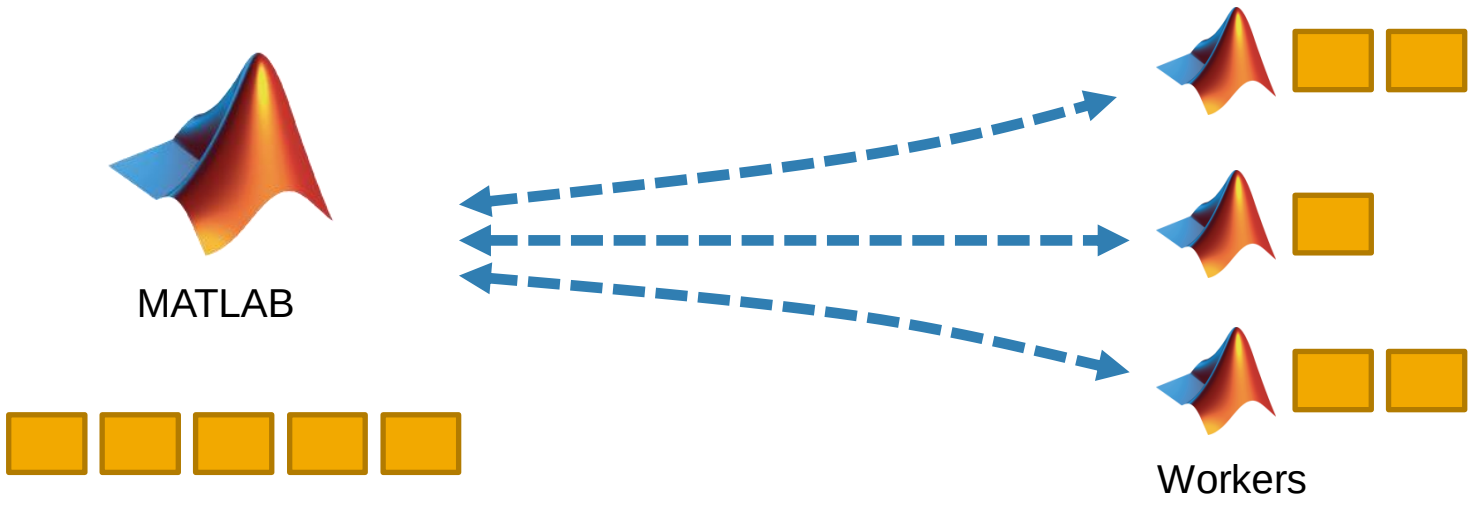
- Run iterations in parallel
- Examples: parameter sweeps, Monte Carlo simulations



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: Convert a simple `for` to `parfor`

Getting Started with `parfor`

In this exercise, we will convert 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
```

```
     1

     2

     3
```

Common problems when you try to convert `for`-loops to `parfor`-loops

! Noninteger loop variables

```
parfor x = 0:0.1:1
    parfor y = 2:10
        A(y) = A(y-1) + y;
    end
end
```

! Nested parallel loops

! Dependent loop body

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 → You might need to modify your code to use `parfor`!

```
1   a = zeros(5,1);
2   b = pi;
3   parfor i = 1:5
4       a(i) = i + b;
5   end
6   disp(a)
```

No warnings found.

```
1   a = zeros(5,1);
2   b = pi;
3   parfor i = 1:5
4       a(i) = a(i-1) + b;
5   end
6   disp(a)
```

Line 3: The PARFOR loop cannot run due to the way variable 'a' is used. Details ▾

Hands-On Exercise: Convert `for`-loops into `parfor`-loops

Convert for-Loops Into parfor-Loops

In some cases, you must modify the code to convert `for`-loops to `parfor`-loops. These example focus on diagnosing and fixing `parfor`-loop problems

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

Ensure parfor-loop variables are consecutive increasing integers

Correct the following `parfor`-loop to make sure the loop variables are consecutive increasing integers.

Hint: You can fix these errors by converting the loop variables into a valid range.

```
parfor x = 0:0.1:1
    disp(x)
end
```

Ensure there are no nested parfor-loops

You cannot nest a `parfor`-loop inside another `parfor`-loop. The reason is that the workers in a parallel pool cannot start or access

Because parallel processing incurs overhead, you must choose carefully whether you want

loop

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 ☹

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

Check mathworks.com/help/parallel-computing/improve-parfor-performance.html for ways to improve **`parfor`** performance.

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

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

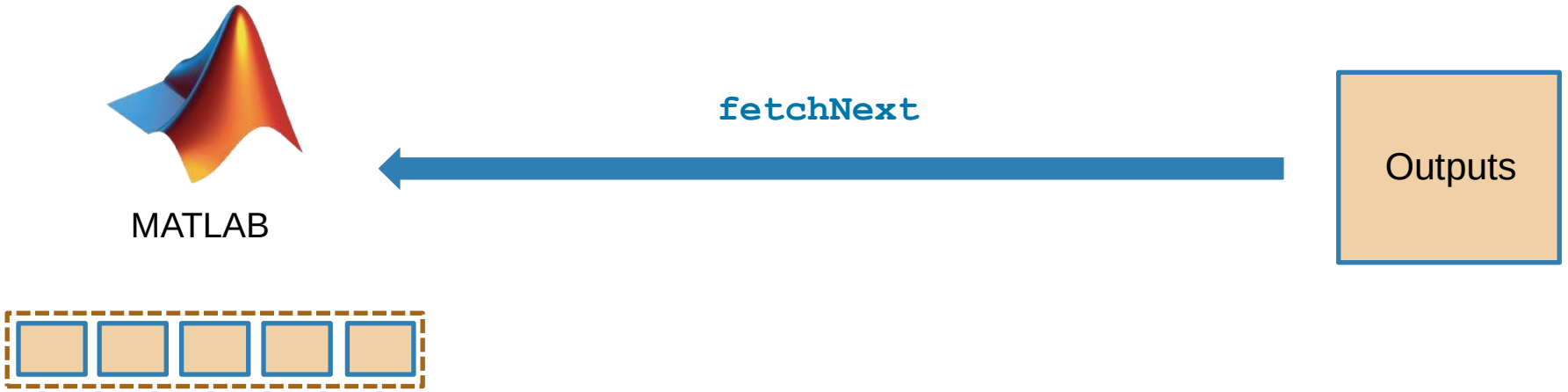
Asynchronously with `parfeval`*

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

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

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

* Runs **function** on parallel workers

Execute functions in parallel asynchronously using `parfeval`



Asynchronous execution on parallel workers

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

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

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

Getting Started with `parfeval`

This exercise shows how to use `parfeval` to run functions in the background.

Set up parallel environment

Create a parallel pool `p` with two workers.

```
clear
delete(gcp('nocreate'))
p = parpool(2);
```

```
Starting parallel pool (parpool) using the 'local' profile ...
Connected to the parallel pool (number of workers: 2).
```

Add work to queue

When you use `parfeval` to run functions in the background, this creates an object called *future* for each function and adds the object to the pool queue.

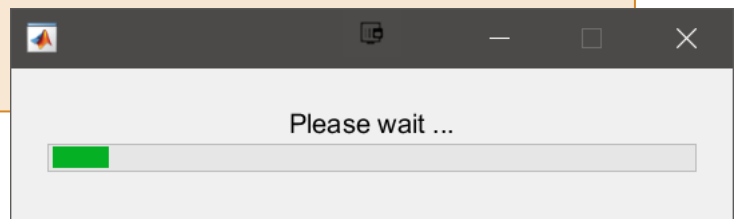
Let's use `parfeval` by instructing workers to execute the function `pause(1)` twice, thus simulating two com
each take one second to compute.

- The inputs to `parfeval` are the function handle (@) to th

Execute additional code as `parfor/parfeval` 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
```



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

Execute additional code as `parfeval` iterations complete

When you offload computations to workers using `parfeval`, you can use `afterEach` and `afterAll` to automatically invoke functions on each or all of the results of `parfeval` computations.

Call `afterEach` on `parfeval` computations

Let's use `parfeval` to compute random vectors in the workers, and `afterEach` to display the largest element in each of those vectors after they are created. `afterEach` executes the function handle on the output of each future when they become ready.

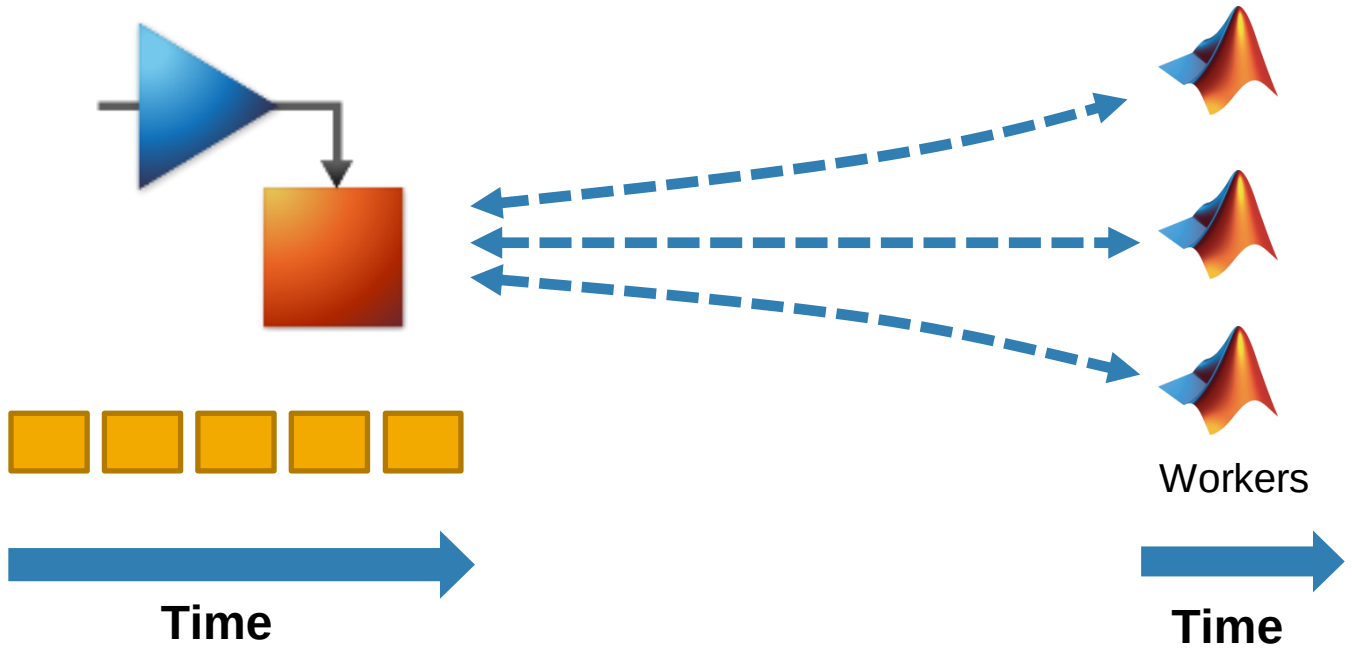
```
p = gcp;
```

```
Starting parallel pool (parpool) using the 'local' profile ...
Connected to the parallel pool (number of workers: 4).
```

```
numOutputs = 1;
input1 = 1e6;
input2 = 1;
f(1:10) = parallel.FevalFuture;
for idx = 1:10
    f(idx) = parfeval(@rand, numOutputs, input1, input2);
end
```

Use `afterEach` to compute the largest elements of these vectors as

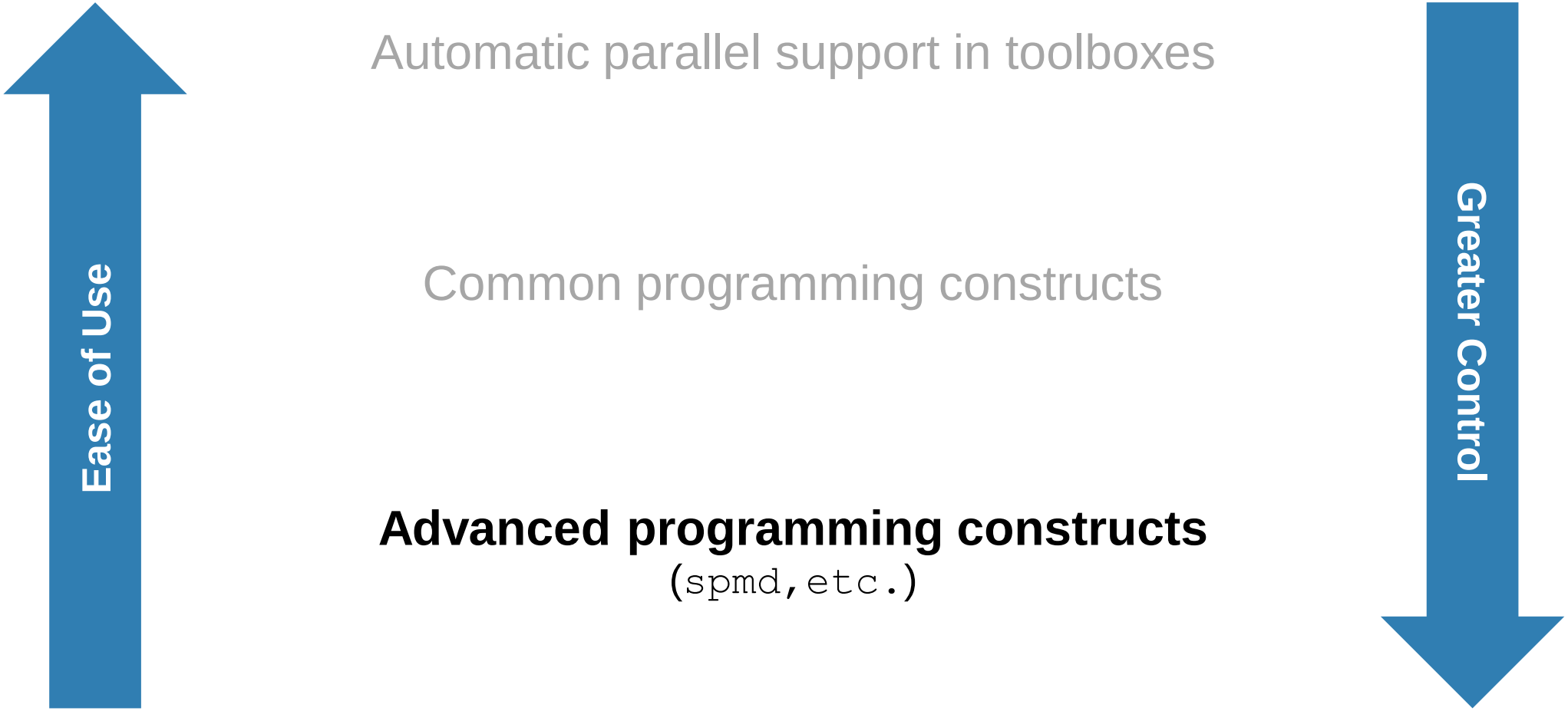
Run multiple simulations in parallel with `parsim`



- 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);
```

Scaling MATLAB applications and Simulink simulations



SPMD: communicating parallel computations with full control

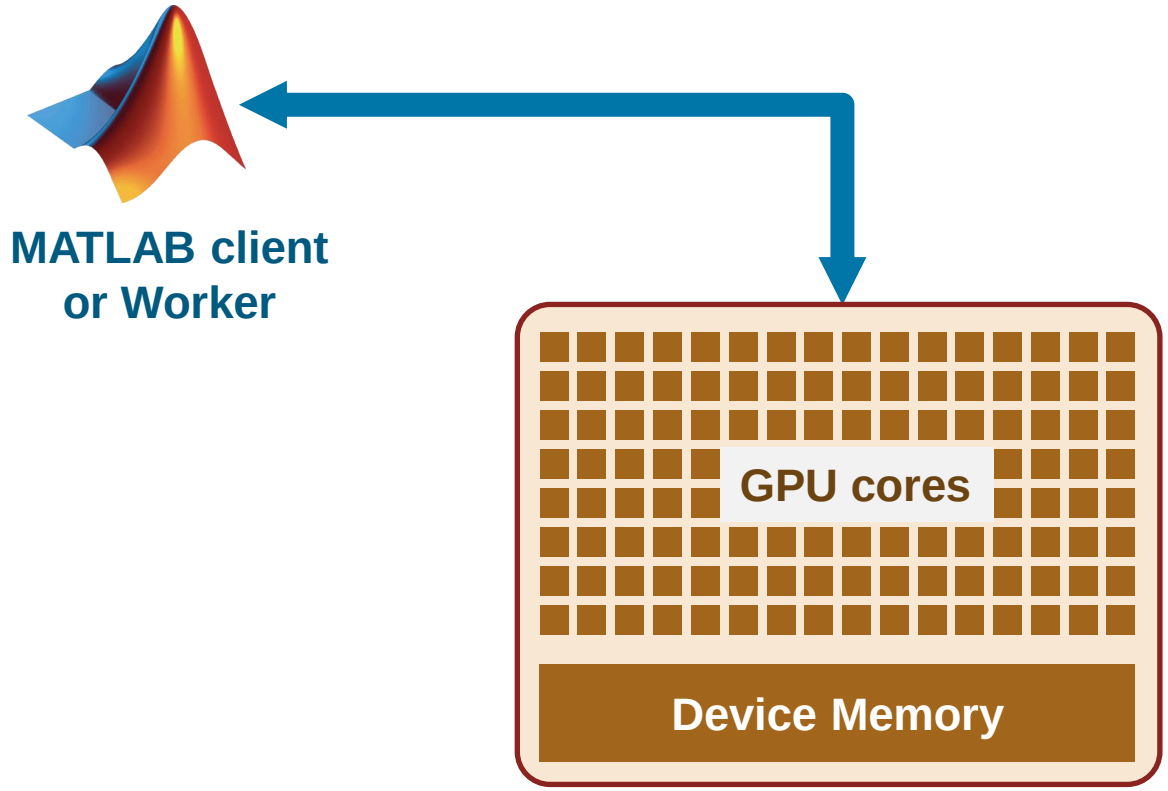
```
spmd
    if spmdIndex==1
        disp("I am 1, sending messages!")
        spmdSend("Message from 1 to 4",4);
        spmdSend("Message from 1 to 3",3);
        spmdSend("Message from 1 to 2",2);
    else
        disp("I am " + num2str(spmdIndex) + ", receivin
        m = spmdReceive("any");
        disp(m);
    end
end
```

```
Worker 1:
  I am 1, sending messages!
Worker 2:
  I am 2, receiving:
  Message from 1 to 2
Worker 3:
  I am 3, receiving:
  Message from 1 to 3
Worker 4:
  I am 4, receiving:
  Message from 1 to 4
>>
```

- The **spmd** block allows communicating parallel code execution, where each worker can run different code or operate on different data
- **spmd** in MATLAB is conceptually similar to MPI (Message Passing Interface) as both allow for parallel execution across multiple processors or nodes and support explicit communication between processes

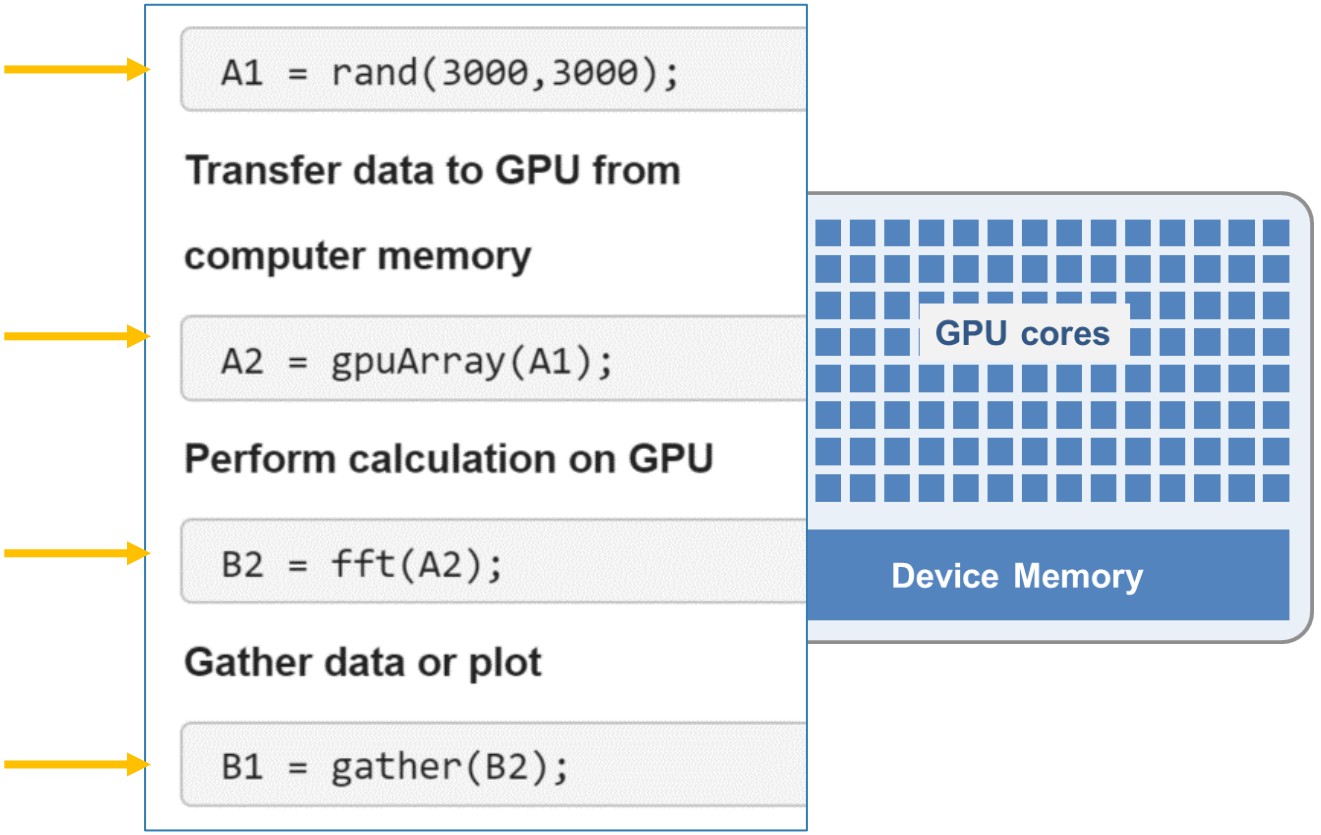
https://www.mathworks.com/help/parallel-computing/spmd.html

Using NVIDIA GPUs with the Parallel Computing Toolbox



Leverage your GPU to accelerate your MATLAB code

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



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

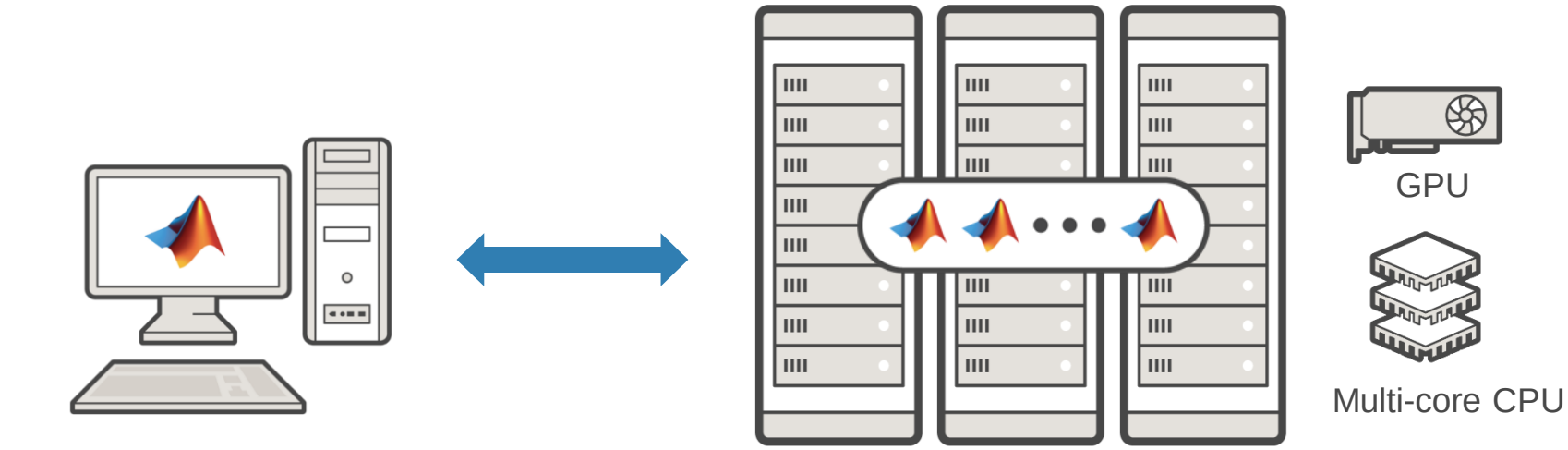
Compute the `fft` on a random matrix:

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

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

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

```
FFT time on CPU: 0.24305
```

...ur GPU device

Parallel computing on your desktop, clusters, and clouds



MATLAB
Parallel Computing Toolbox

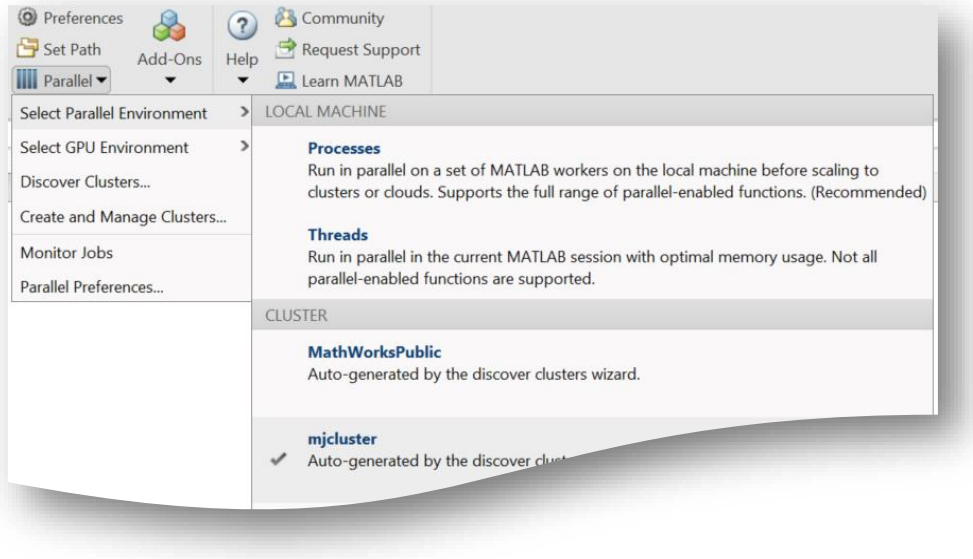
MATLAB Parallel Server

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

Scale to clusters and clouds

With MATLAB Parallel Server, you can…

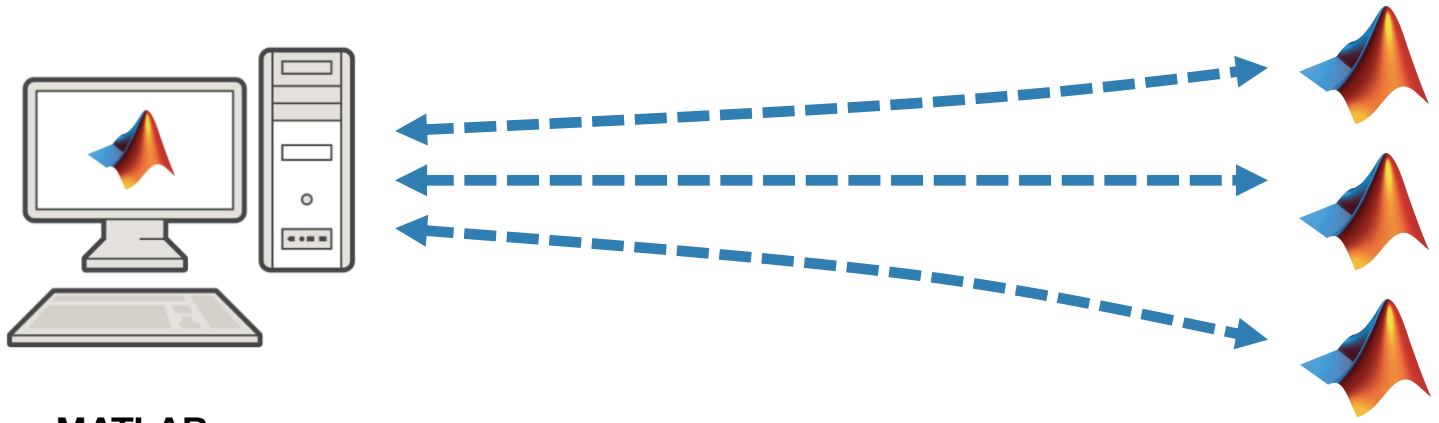
- Change hardware with minimal code change
- Submit to on-premise or cloud clusters
- Support cross-platform submission
  - Windows client to Linux cluster



Interactive parallel computing

Leverage cluster resources in MATLAB

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

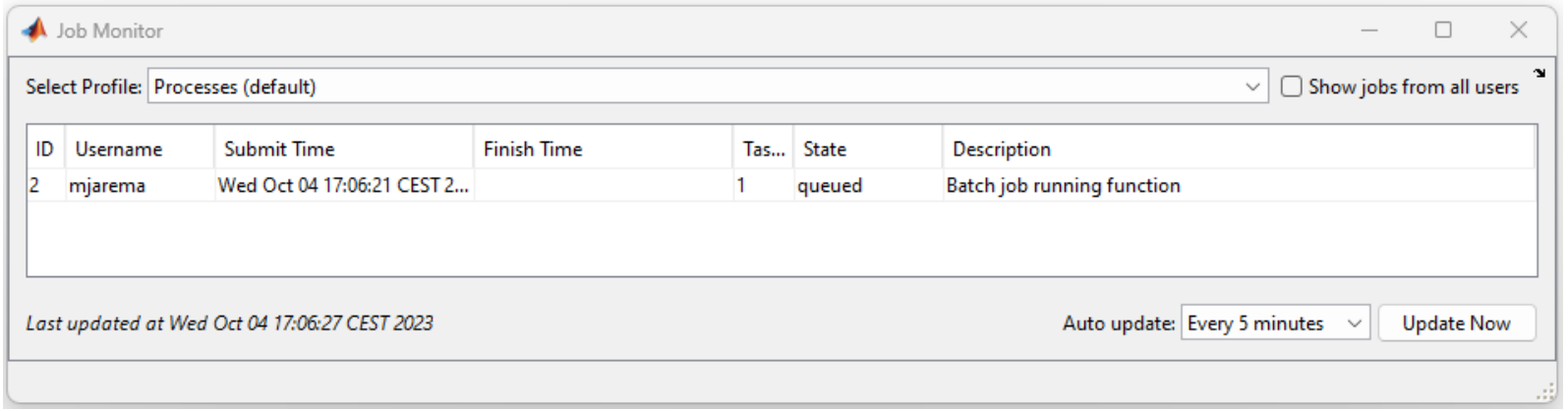


MATLAB

Parallel Computing Toolbox

myscript.m:

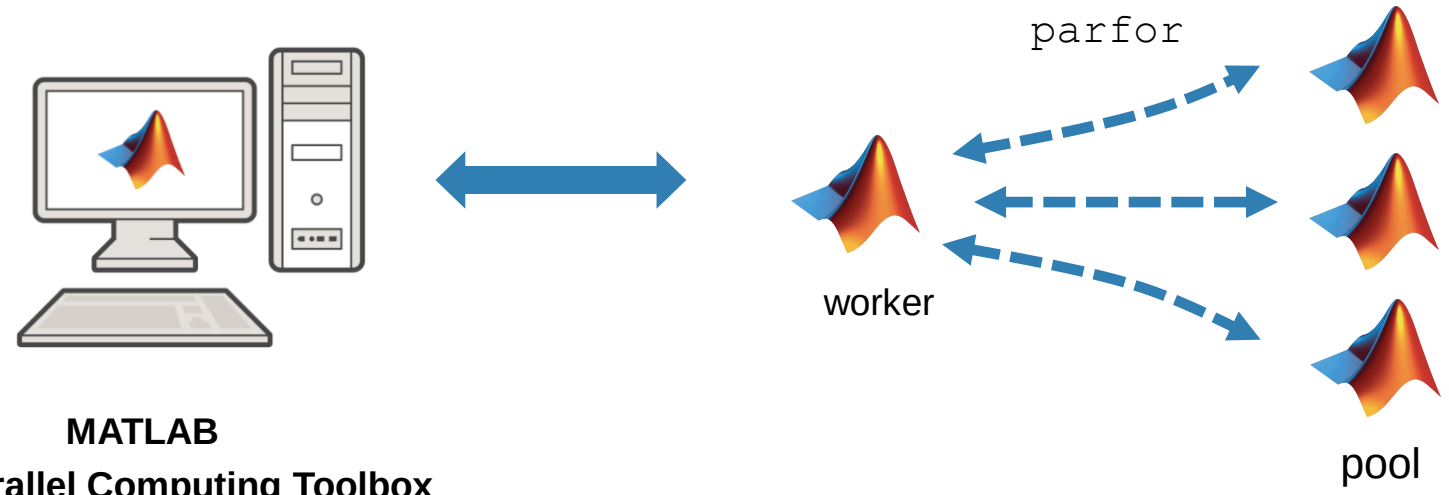
```
a = zeros(5, 1);
b = pi;
parfor i = 1:5
   a(i) = i + b;
end
```



`batch` simplifies offloading computations

Submit MATLAB jobs to the cluster

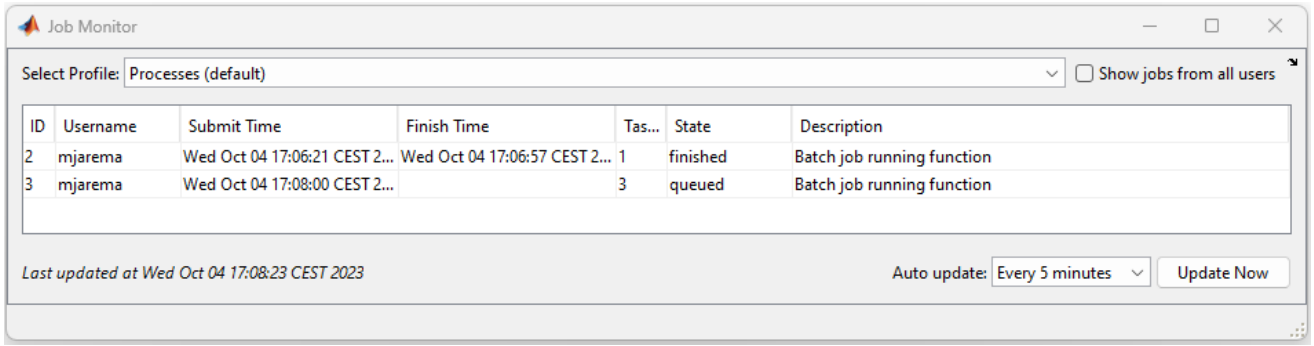
```
>> job = batch('myscript','Pool',3);
```



MATLAB

Parallel Computing Toolbox

```
>> j.State
ans =
    'running'
>> j.diary
Warning: The diary of this batch job might be incomplete
because the job is still running.
--- Start Diary ---

Analyzed 1 image.
Analyzed 2 images.
Analyzed 3 images.
Analyzed 4 images.

--- End Diary ---
```



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

Getting Started with `batch`

We 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 and we can continue working while computations take place. When we submit batch jobs to another computer or cluster, we can even close MATLAB on the client, and retrieve results later.

In this exercise, we will submit batch jobs from MATLAB to our 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 our local resources.

Run a `batch` job to offload a serial computation

`batch` runs our code on a local worker or a cluster worker, but does not require a parallel pool. Close a parallel pool, if one is open.

```
delete(gcp('nocreate'))
```

Use the batch command to offload the function `ex_serial` to one MATLAB worker session that runs in the background, while we can continue using MATLAB as computations take place.

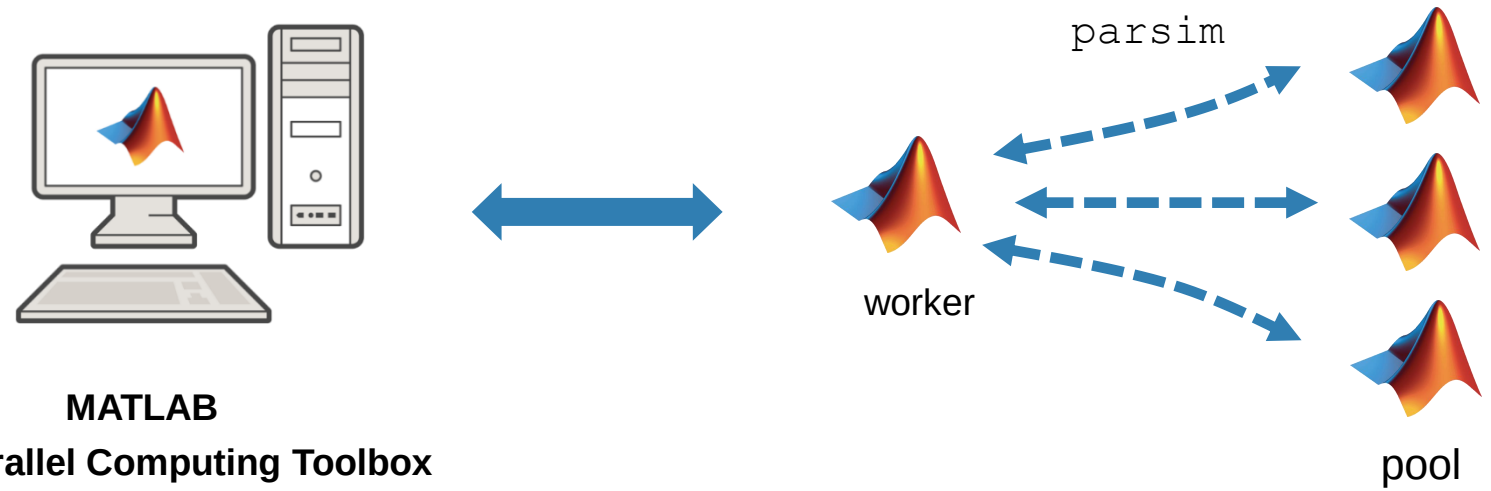
The function performs `N` trials of computing the largest eigenvalue for an `M-by-M` random matrix and run

```
numOutputs = 1;
```

`batch` simplifies offloading simulations

Submit Simulink jobs to the cluster

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



Big Data Workflows

ACCESS DATA

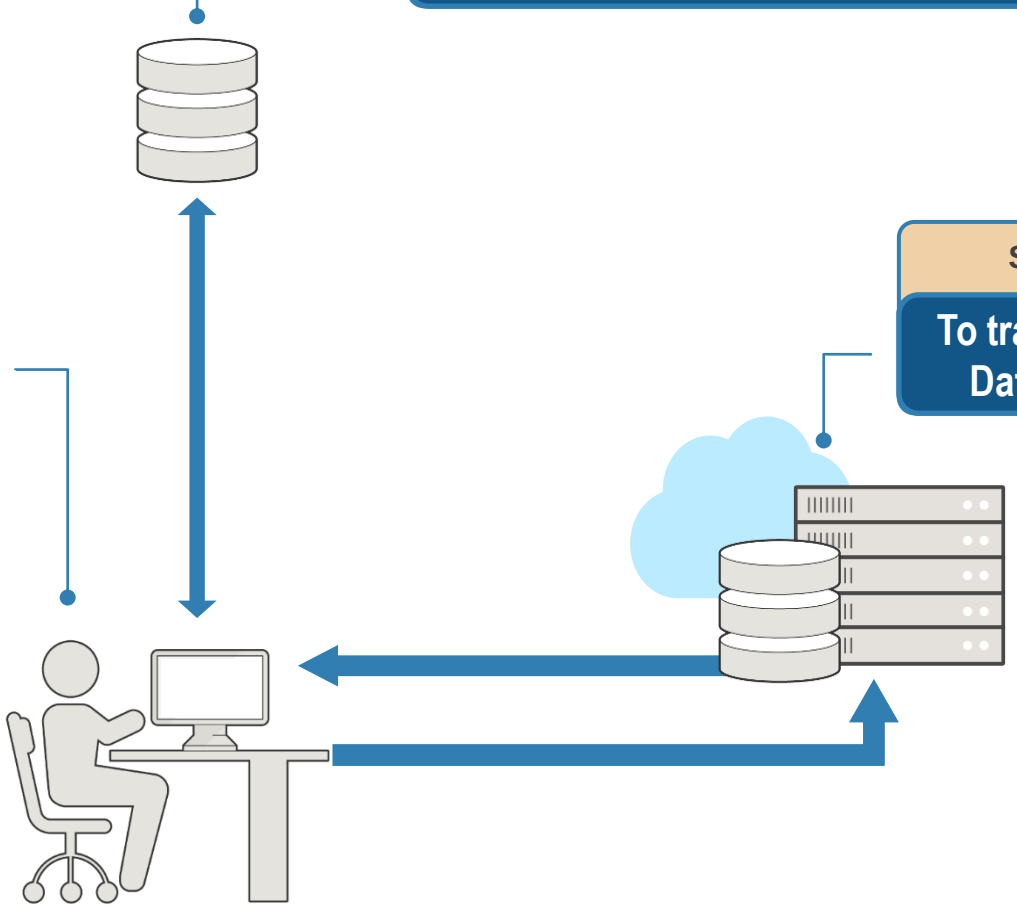
More data and collections of files than fit in memory

DEVELOP & PROTOTYPE ON THE DESKTOP

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

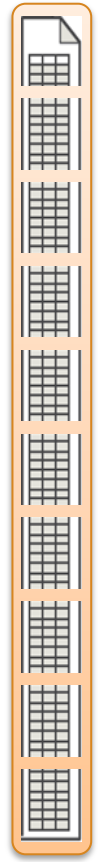
SCALE PROBLEM SIZE

To traditional clusters and Big Data systems like Hadoop



`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.)



[Working with tall arrays]

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.

We can work with many operations and functions as we would with in-memory MATLAB arrays, but most results are evaluated only when we 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)

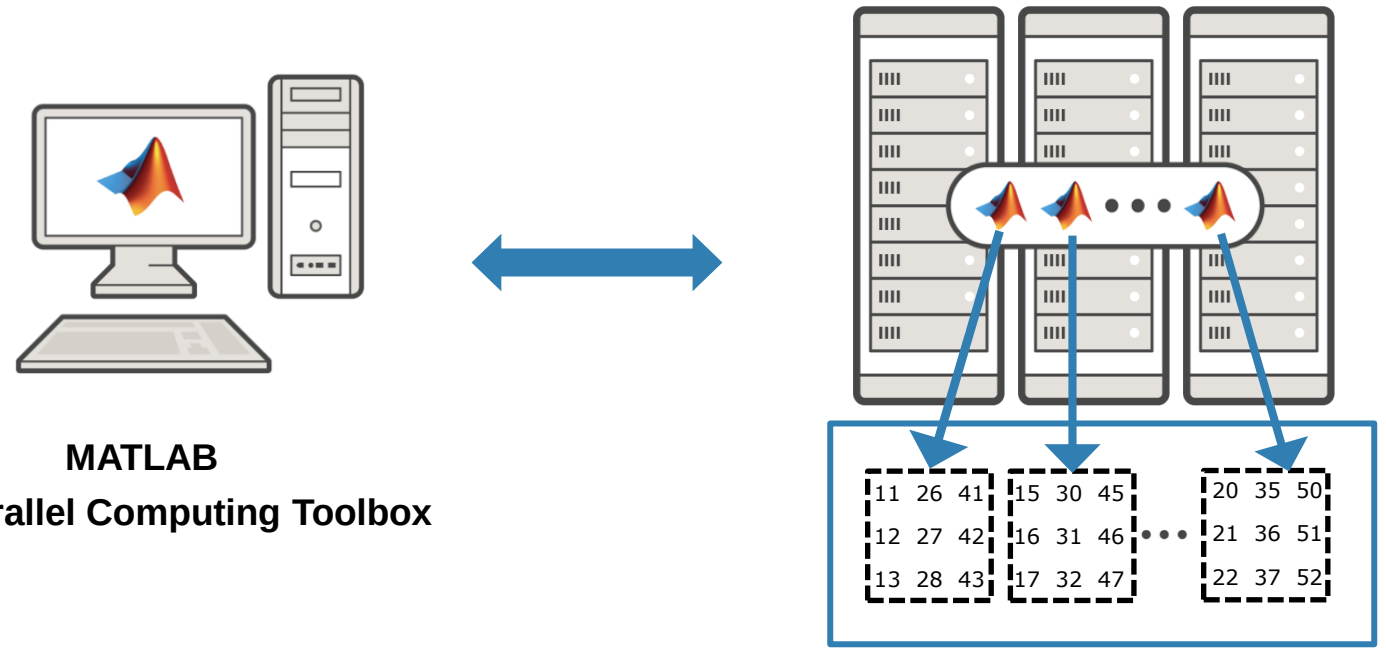
The comma-separated text file `airlinesmall.csv` contains departure and arrival information about individual airline flights from the years 1987 through 2008, stored in a tabular manner.

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 i
programmatically, by reading the comma-separated text fi

`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
- You *can* prototype on desktop, but distributed is only useful on cluster machines.
- Note: **not** designed to increase performance, but to expand memory barriers!

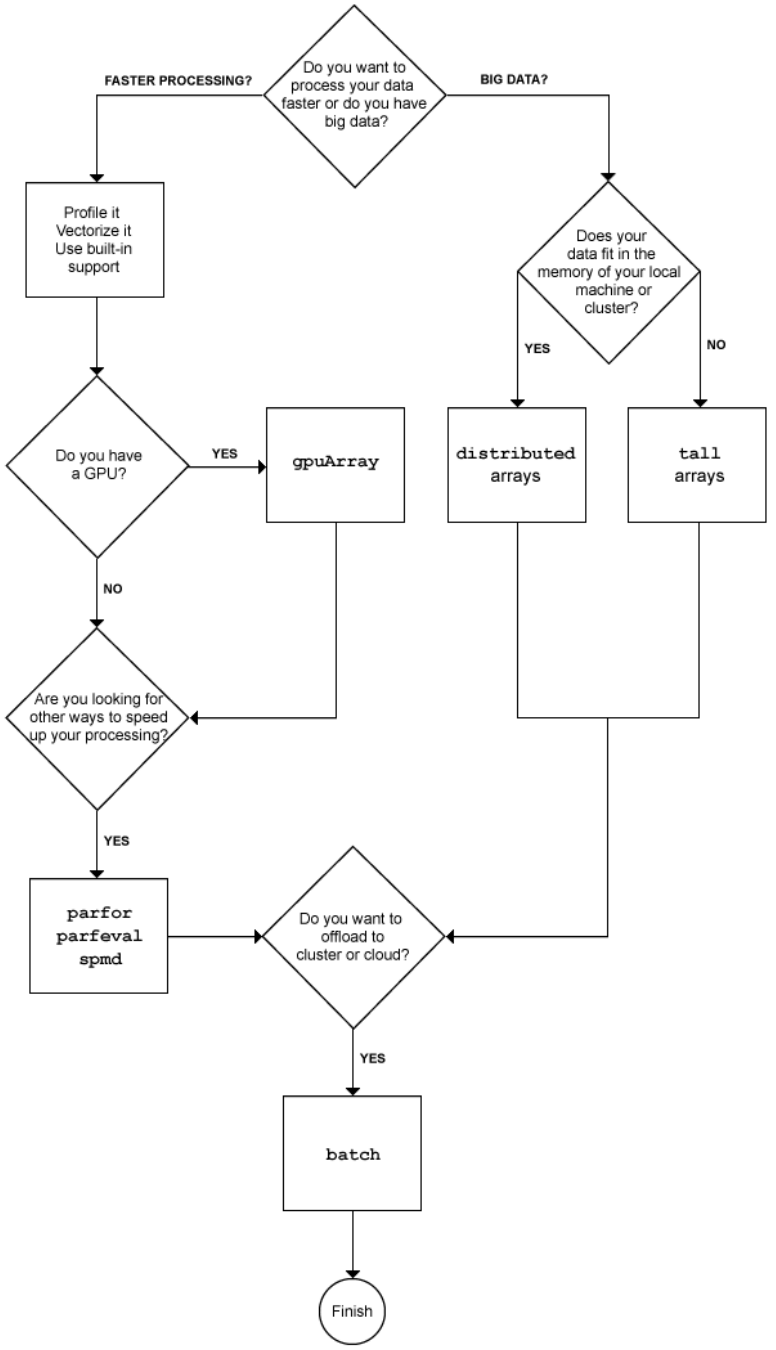


[Working with distributed arrays]

Choose your solution to accelerate your code

Top 5 MATLAB Acceleration Techniques

1. Adopt Efficient (Serial) Programming Practices
2. Leverage Existing Optimized Algorithms
3. Use Parallel Computing including GPUs
4. Use Parallel Computing
5. Generate C Code from MATLAB Code
6. All of the Above



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
  - https://www.mathworks.com/solutions/parallel-computing.html

Survey Link

The survey is for all workshops, so if you plan to attend additional/all workshops of the series, please fill out the survey afterwards

https://forms.office.com/r/MCrysvLtj8