WORKSHOP: Parallel Computing with MATLAB (Part I)

Raymond Norris
Application Engineer, MathWorks
July 21, 2021

Agenda

- Part I – Parallel Computing with MATLAB on the Desktop
  - Parallel Computing Toolbox
  - MATLAB Online
- Part II – Scaling MATLAB to Compute Canada cluster
  - MATLAB Parallel Server
  - VNC

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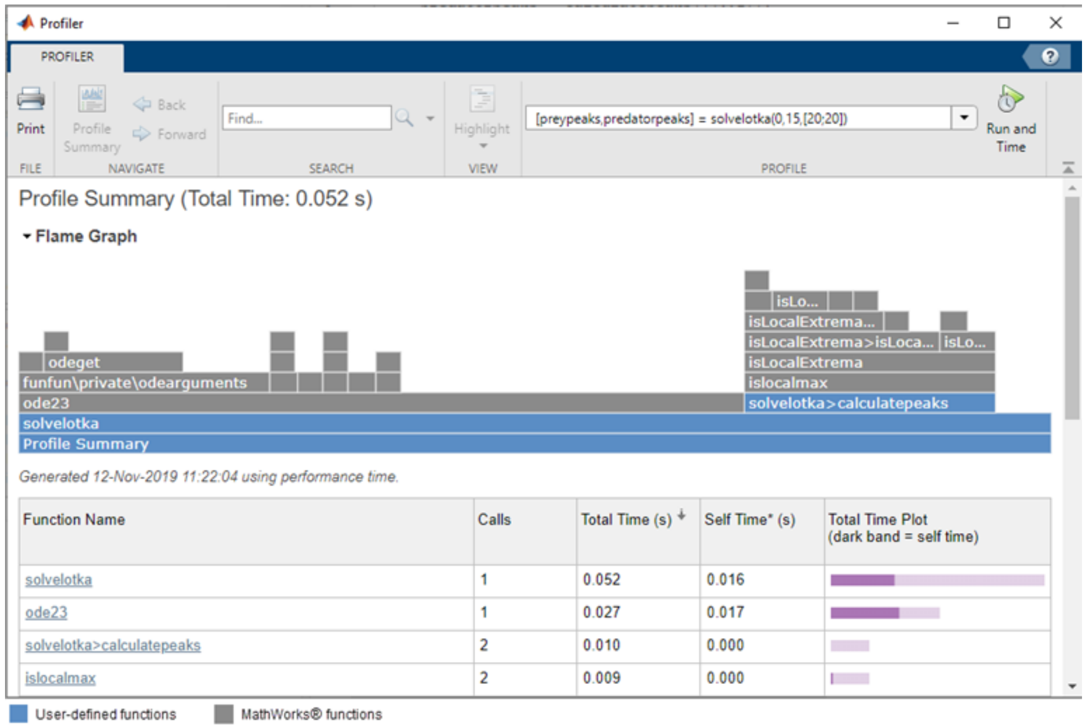
- Part I – Parallel Computing with MATLAB on the Desktop
  - Parallel Computing Toolbox
  - MATLAB Online
- Part II – Scaling MATLAB to Compute Canada cluster
  - MATLAB Parallel Server
  - VNC

Save time and tackle increasingly complex problems

- Reduce computation time by using available compute cores and GPUs
- Scale and accelerate workflows with minimal code changes
- Scale computations to clusters and clouds
- Focus on your engineering and research, not the computation

Optimize your code before parallelizing for best performance

- Find bottlenecks with profiler



[preypeaks,predatorpeaks] = solvelotka(0,15,[20;20])

Profile Summary (Total Time: 0.052 s)

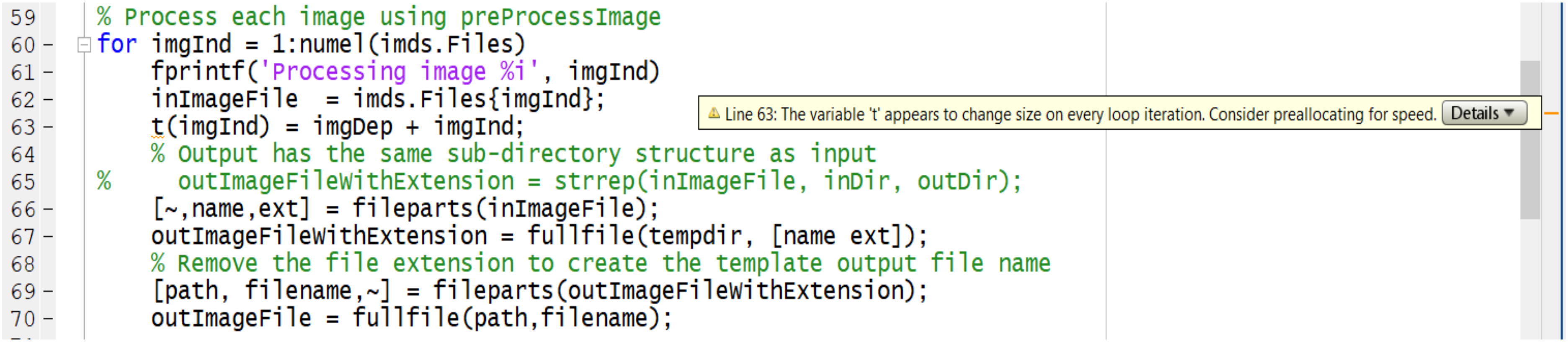
Generated 12-Nov-2019 11:22:04 using performance time.

Function Name	Calls	Total Time (s)	Self Time* (s)	Total Time Plot (dark band = self time)
solvelotka	1	0.052	0.016	
ode23	1	0.027	0.017	
solvelotka>calculatepeaks	2	0.010	0.000	
islocalmax	2	0.009	0.000	

Techniques for accelerating MATLAB algorithms and applications

Optimize your code before parallelizing for best performance

- Implement effective programming techniques



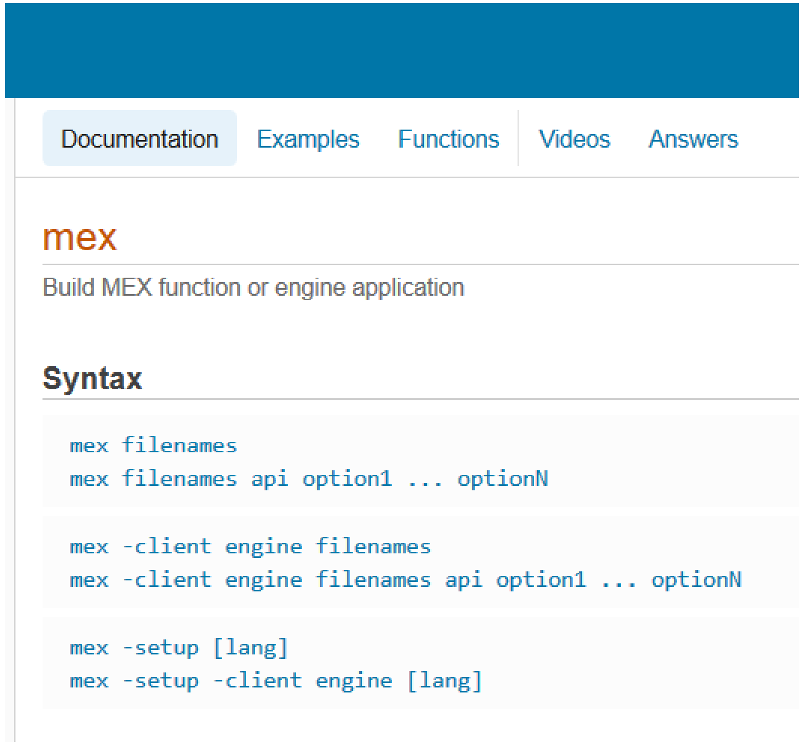
```
59      % Process each image using preProcessImage
60 -  for imgInd = 1:numel(imds.Files)
61 -      fprintf('Processing image %i', imgInd)
62 -      inImageFile  = imds.Files{imgInd};
63 -      t(imgInd) = imgDep + imgInd;
64        % Output has the same sub-directory structure as input
65    %    outImageFileWithExtension = strrep(inImageFile, inDir, outDir);
66 -      [~,name,ext] = fileparts(inImageFile);
67 -      outImageFileWithExtension = fullfile(tempdir, [name ext]);
68        % Remove the file extension to create the template output file name
69 -      [path, filename,~] = fileparts(outImageFileWithExtension);
70 -      outImageFile = fullfile(path,filename);
```

⚠ Line 63: The variable 't' appears to change size on every loop iteration. Consider preallocating for speed.

Techniques for accelerating MATLAB algorithms and applications

Optimize your code before parallelizing for best performance

- (Advanced) Replace code with MEX functions



mex

Build MEX function or engine application

Syntax

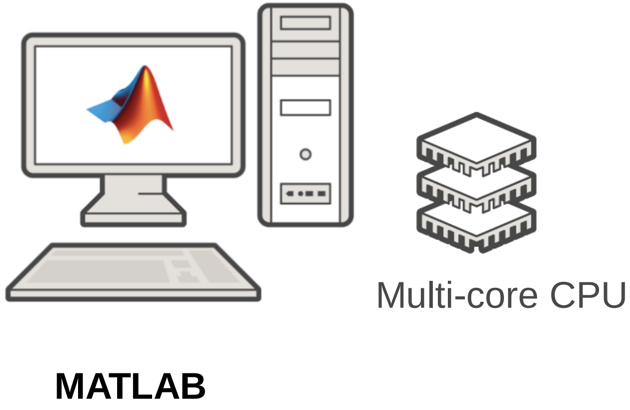
```
mex filenames
mex filenames api option1 ... optionN
```

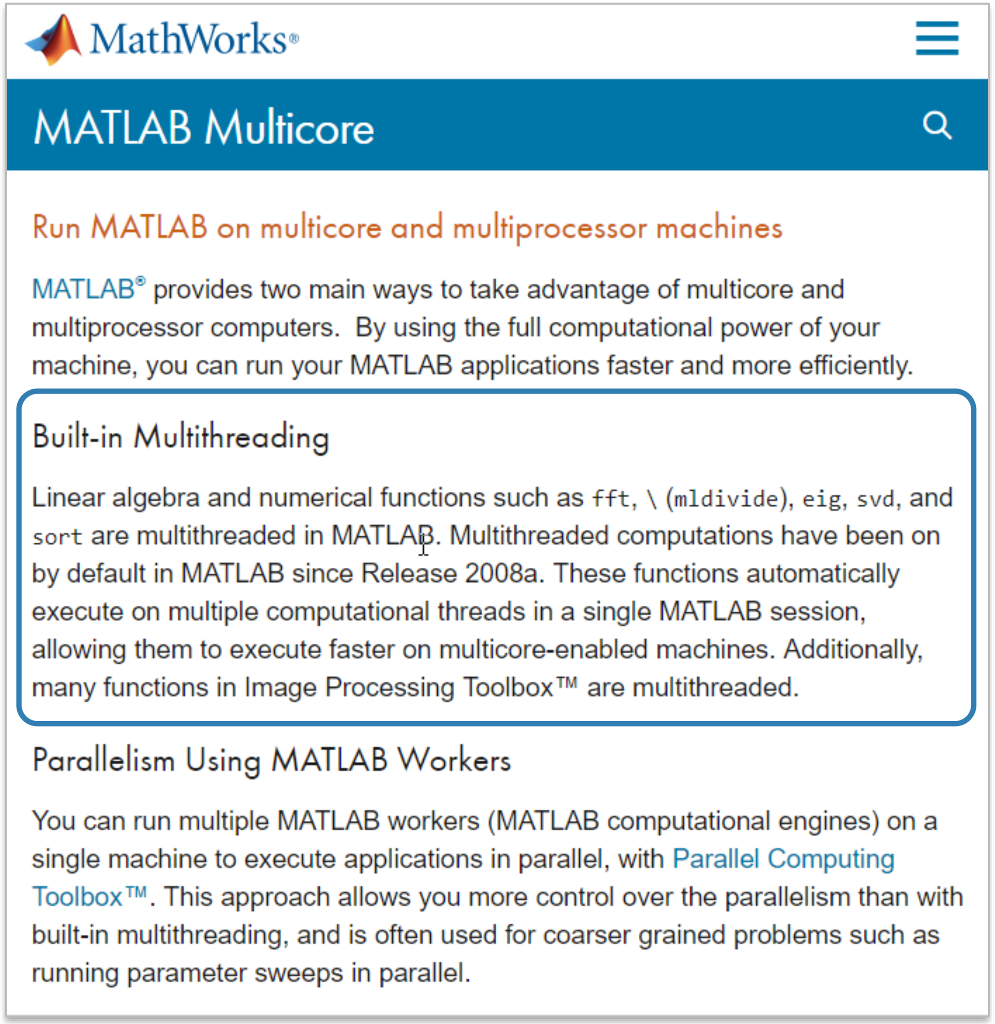
```
mex -client engine filenames
mex -client engine filenames api option1 ... optionN
```

```
mex -setup [lang]
mex -setup -client engine [lang]
```

Techniques for accelerating MATLAB algorithms and applications

MATLAB has built-in multithreading





MathWorks®

MATLAB Multicore

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

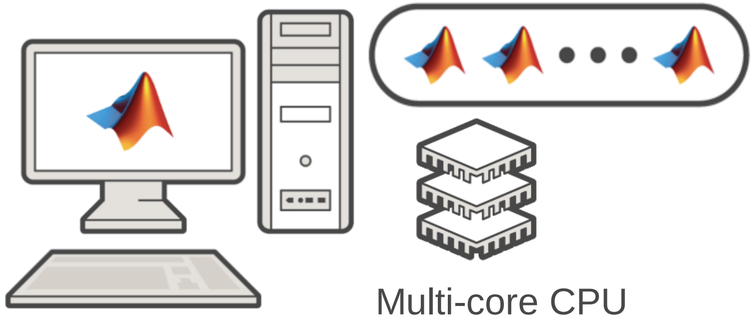
Linear algebra and numerical functions such as `fft`, `\` (`mldivide`), `eig`, `svd`, and `sort` are multithreaded in MATLAB. Multithreaded computations have been on by default in MATLAB since Release 2008a. These functions automatically execute on multiple computational threads in a single MATLAB session,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

Parallelism Using MATLAB Workers

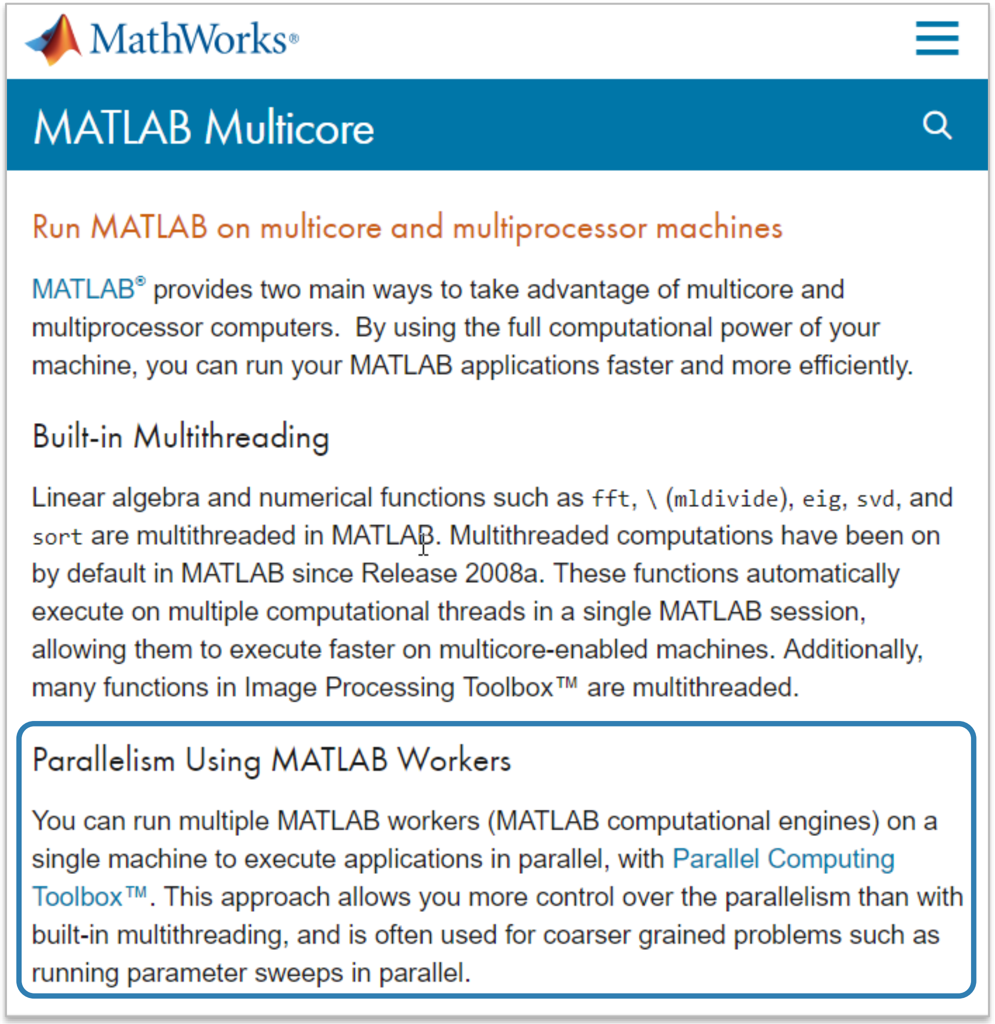
You can run multiple MATLAB workers (MATLAB computational engines) on a single machine to execute applications in parallel, with Parallel Computing Toolbox™. This approach allows you more control over the parallelism than with built-in multithreading, and is often used for coarser grained problems such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

MATLAB multicore

Scale further with parallel computing



MATLAB
Parallel Computing Toolbox



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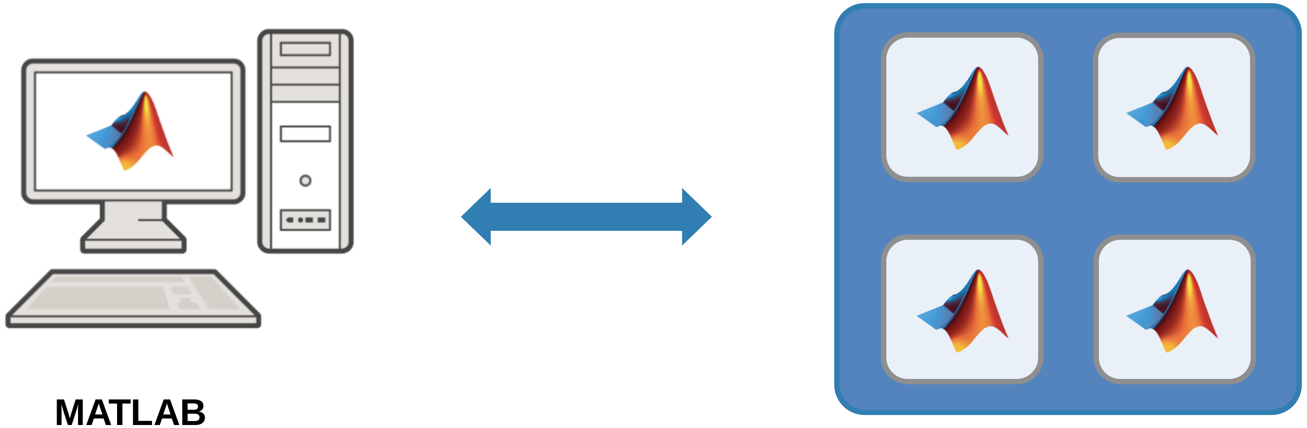
[MATLAB multicore]

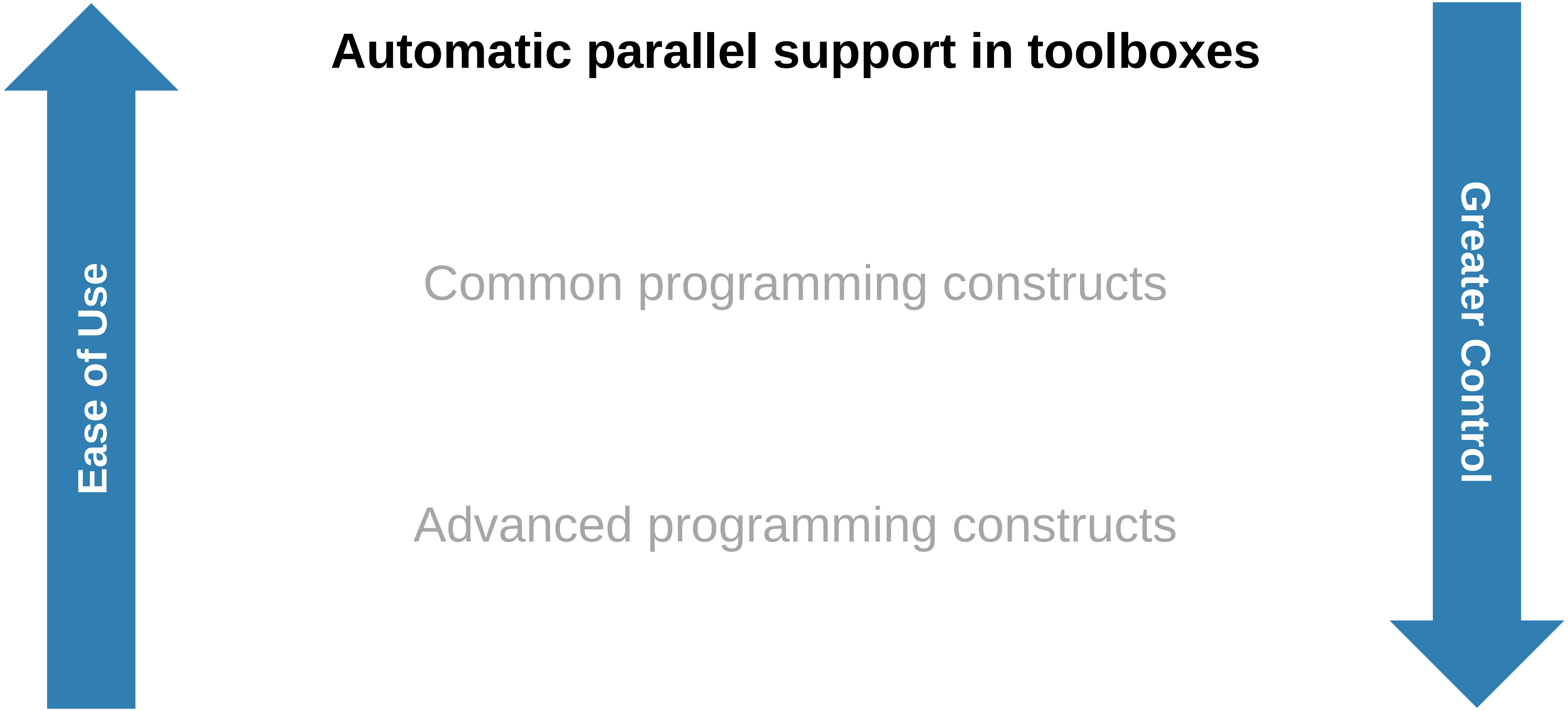
Run multiple iterations by utilizing multiple CPU cores



MATLAB
Parallel Computing Toolbox

Workers

Scaling MATLAB applications and Simulink simulations

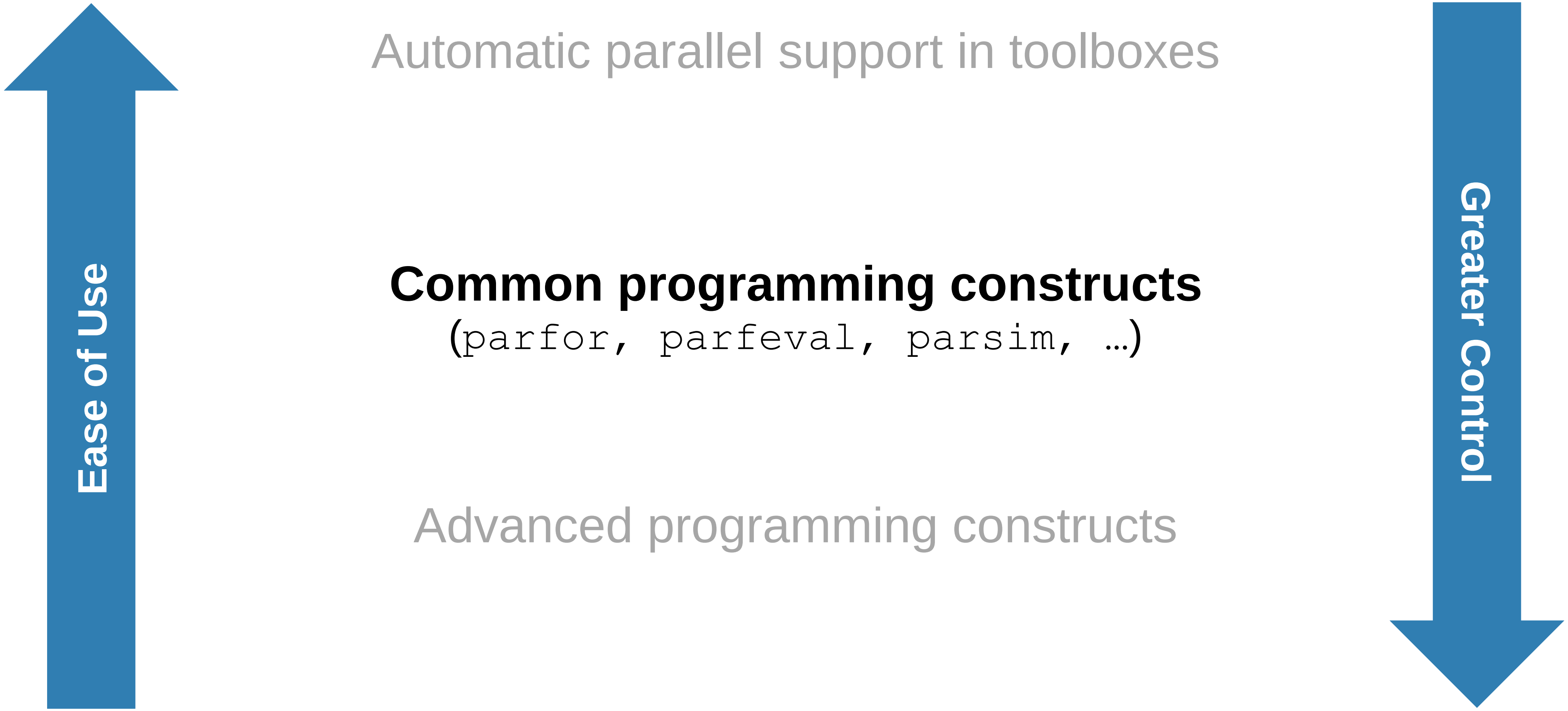


Automatic parallel support in toolboxes

Common programming constructs

Advanced programming constructs

Scaling MATLAB applications and Simulink simulations



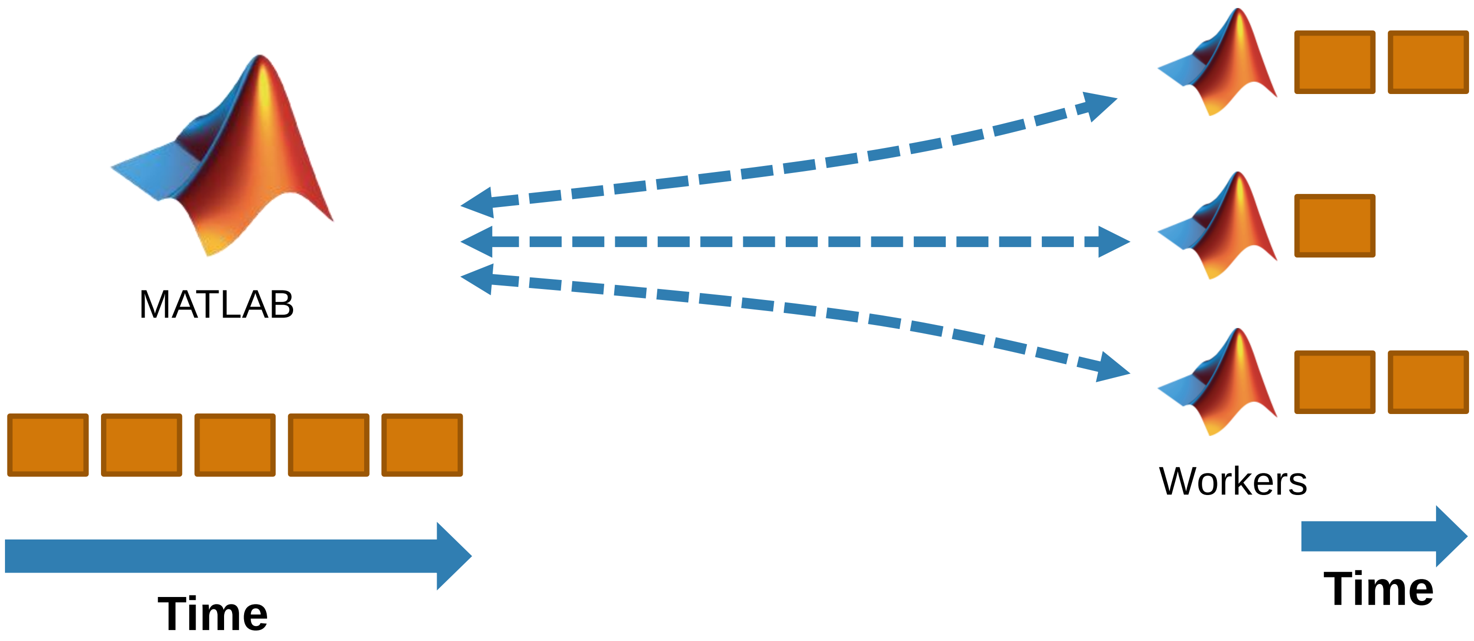
Automatic parallel support in toolboxes

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

Advanced programming constructs

Parallelism using `parfor`

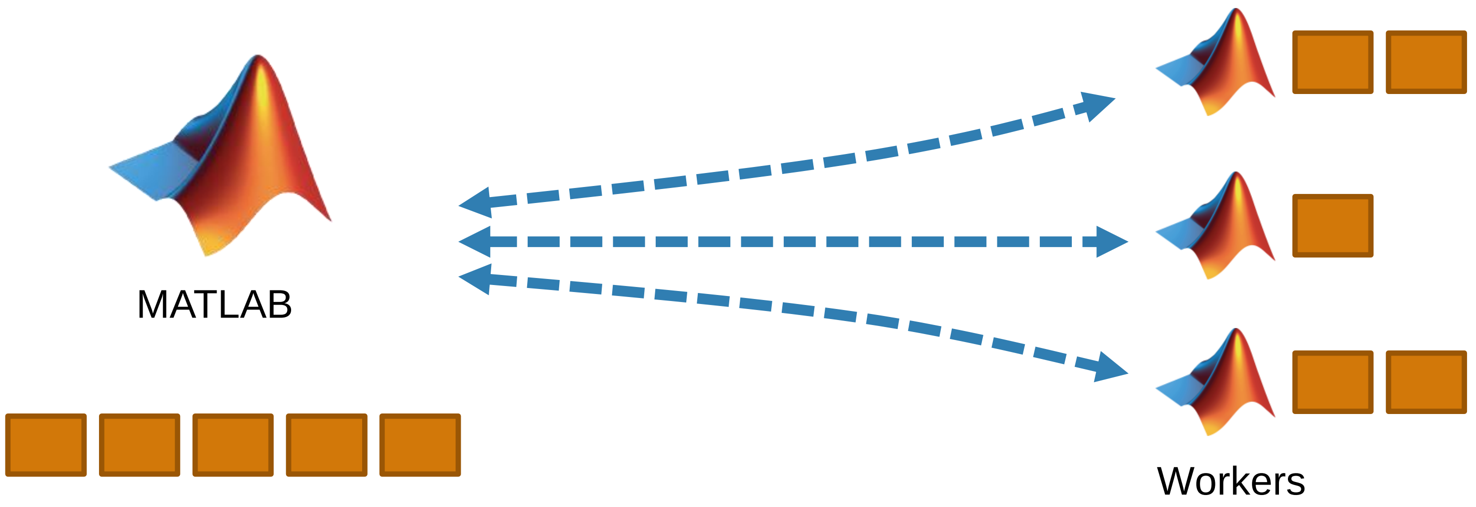
- Run iterations in parallel
- Examples: parameter sweeps, Monte Carlo simulations



Parallelism using `parfor`

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

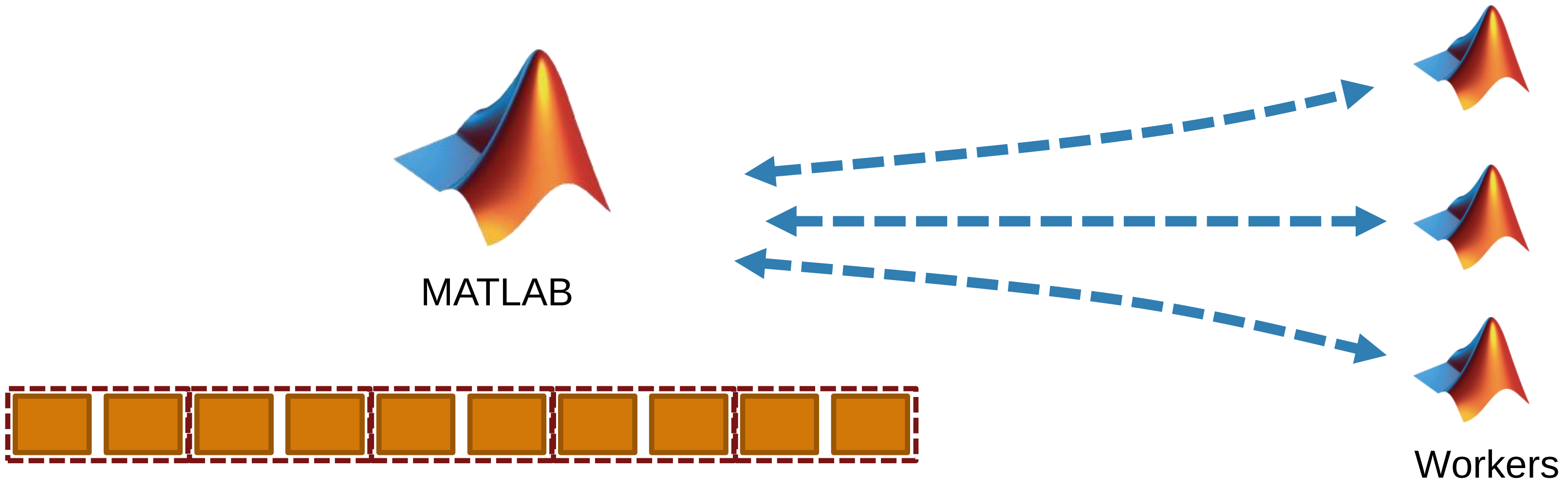
```
a = zeros(5, 1);
b = pi;
parfor i = 1:5
   a(i) = i + b;
end
disp(a)
```



MATLAB

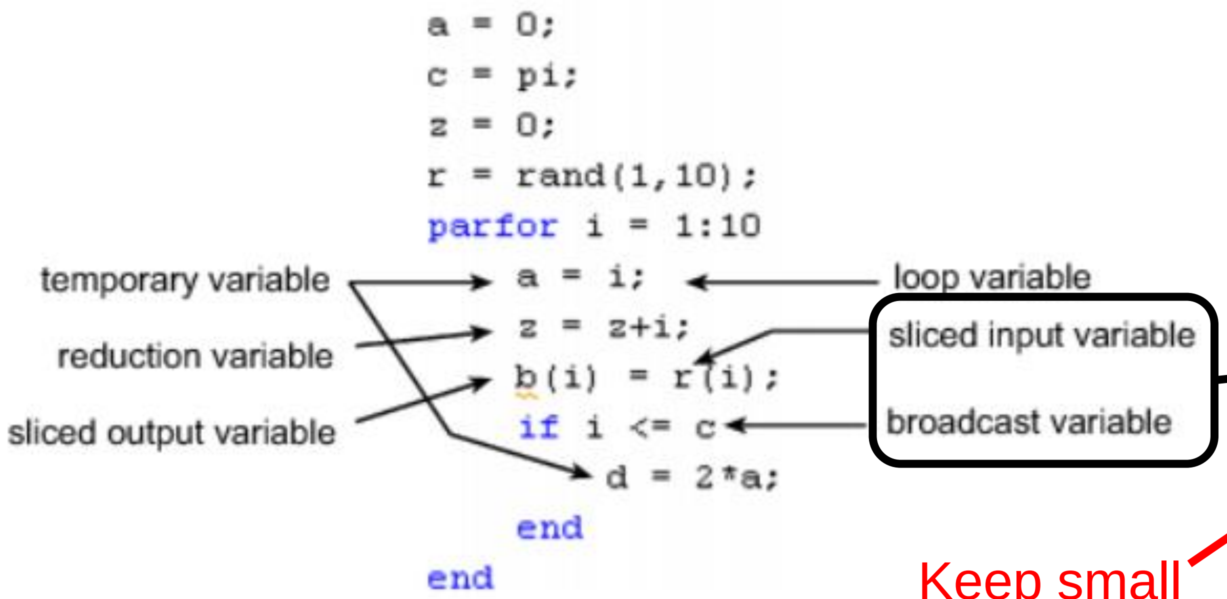
Workers

Parallelize for loops with independent iterations



```
a = zeros(10, 1);
b = pi;
parfor i = 1:10
  a(i) = i + b;
end
disp(a)
```

Optimizing `parfor`



```
a = 0;
c = pi;
z = 0;
r = rand(1,10);
parfor i = 1:10
    a = i;
    z = z+i;
    b(i) = r(i);
    if i <= c
        d = 2*a;
    end
end
```

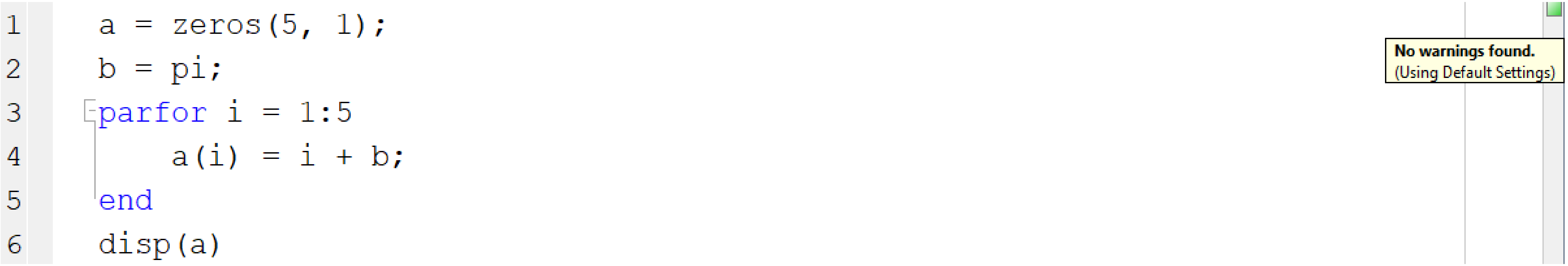
Use more

Keep small

Type	Category
sliced input	input
broadcast	input
reduction	output
sliced output	output
loop	only exist on worker
temporary	only exist on worker

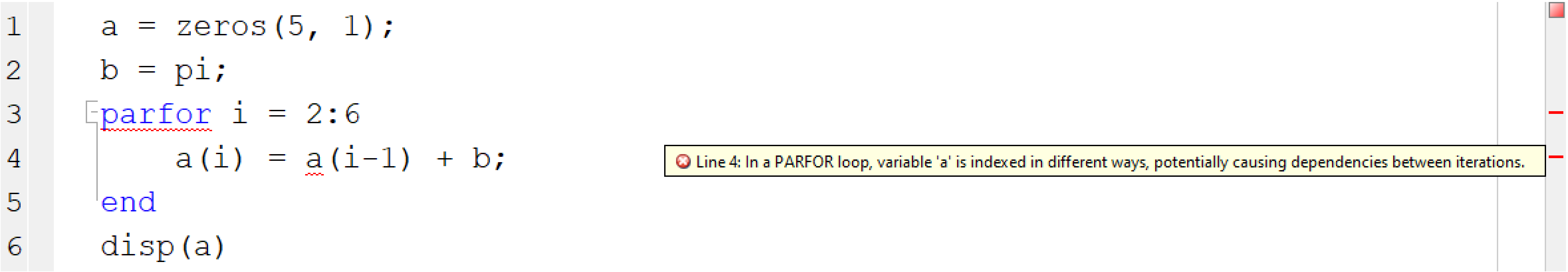
[Troubleshooting variables in parfor-loops]

Parallelism using `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.
(Using Default Settings)



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

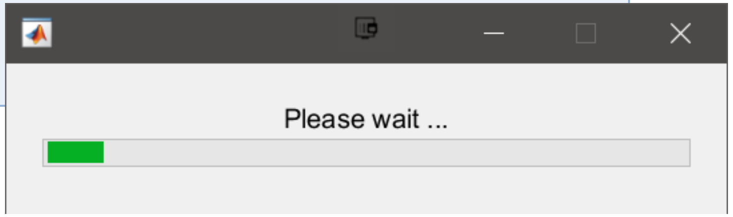
Line 4: In a PARFOR loop, variable 'a' is indexed in different ways, potentially causing dependencies between iterations.

Execute additional code as iterations complete

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

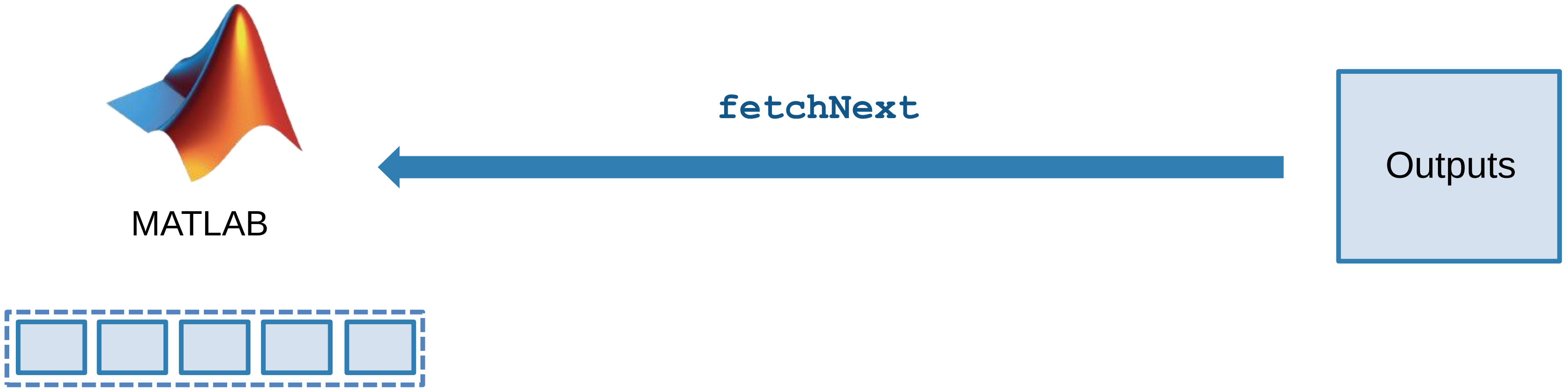
- Retrieve intermediate values and track computation progress

```
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 ...

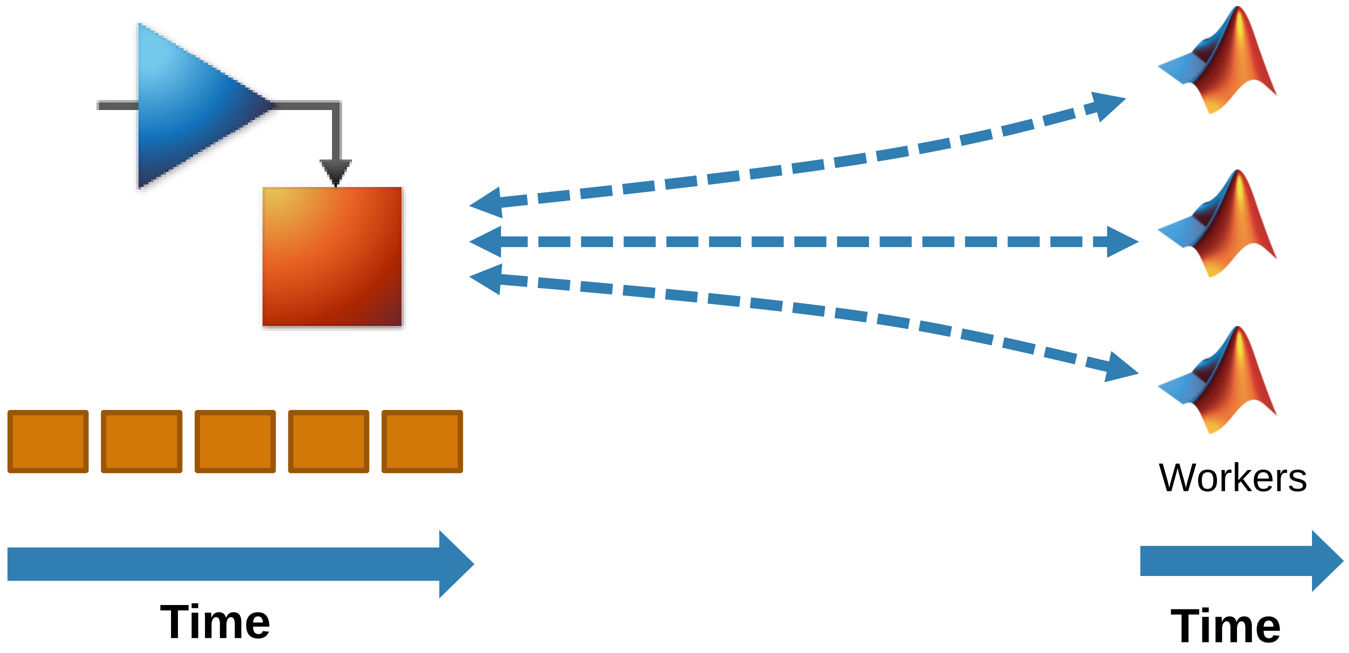
Execute functions in parallel asynchronously using `parfeval`



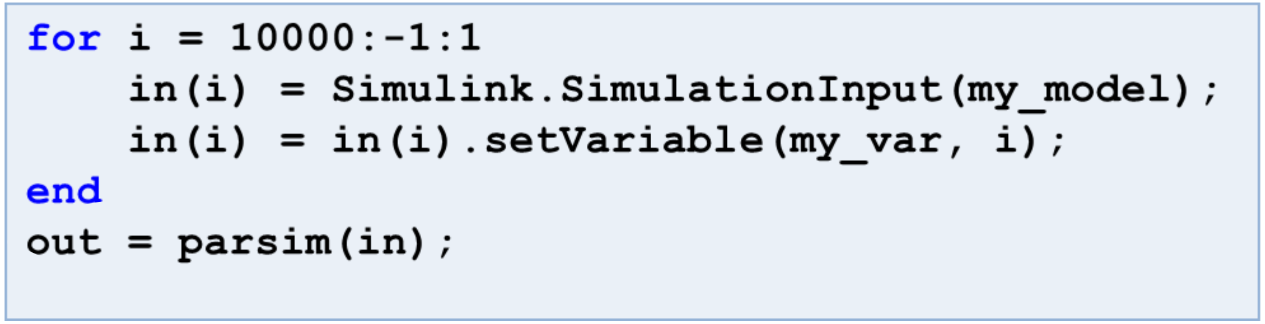
- Asynchronous execution on parallel workers
- Useful for “needle in a haystack” problems

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

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

Run multiple simulations in parallel with `parsim`

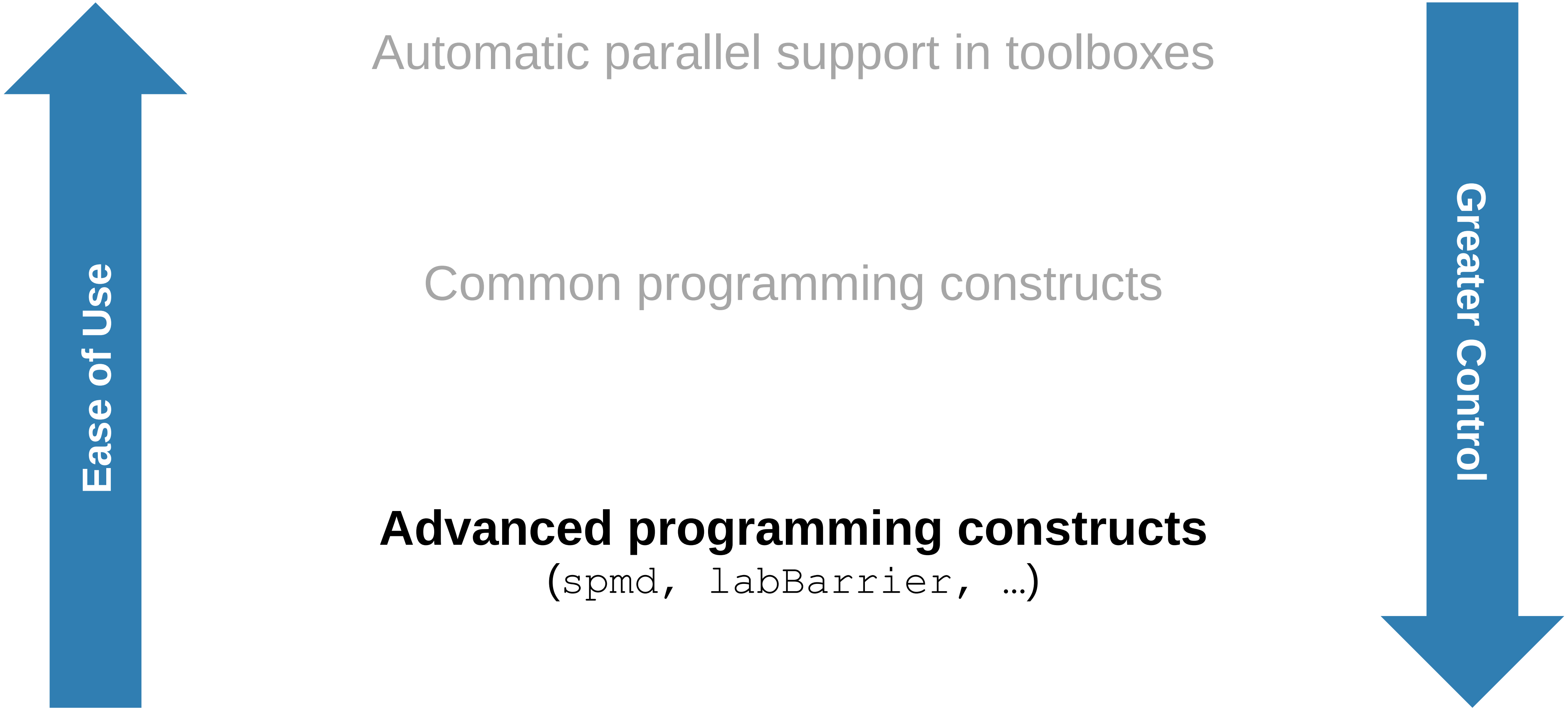


- Run independent Simulink simulations in parallel using the `parsim` function



```
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

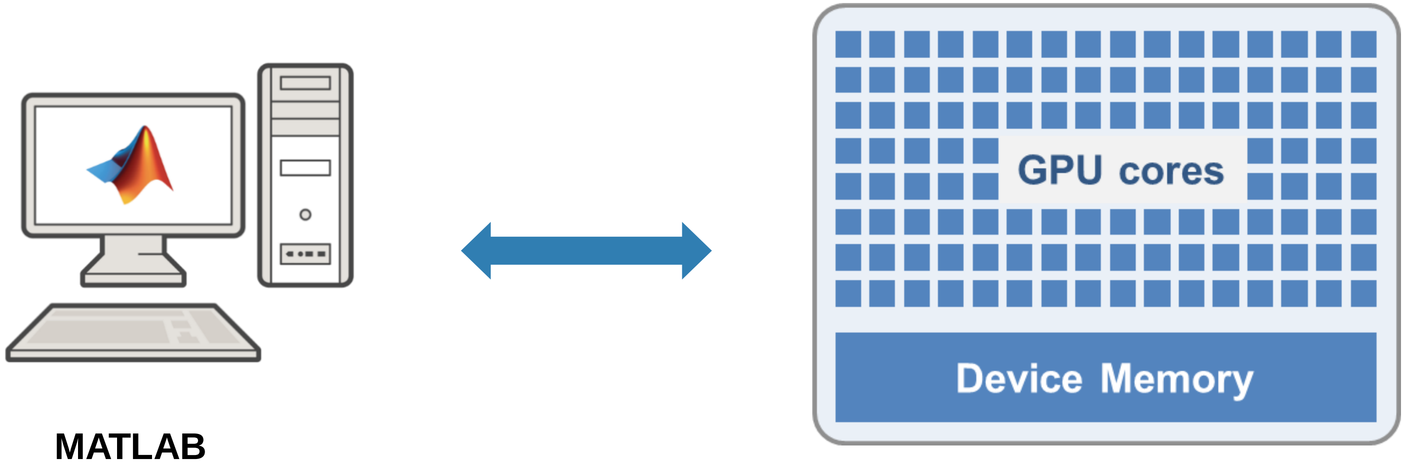


Automatic parallel support in toolboxes

Common programming constructs

Advanced programming constructs
(`spmd, labBarrier, …`)

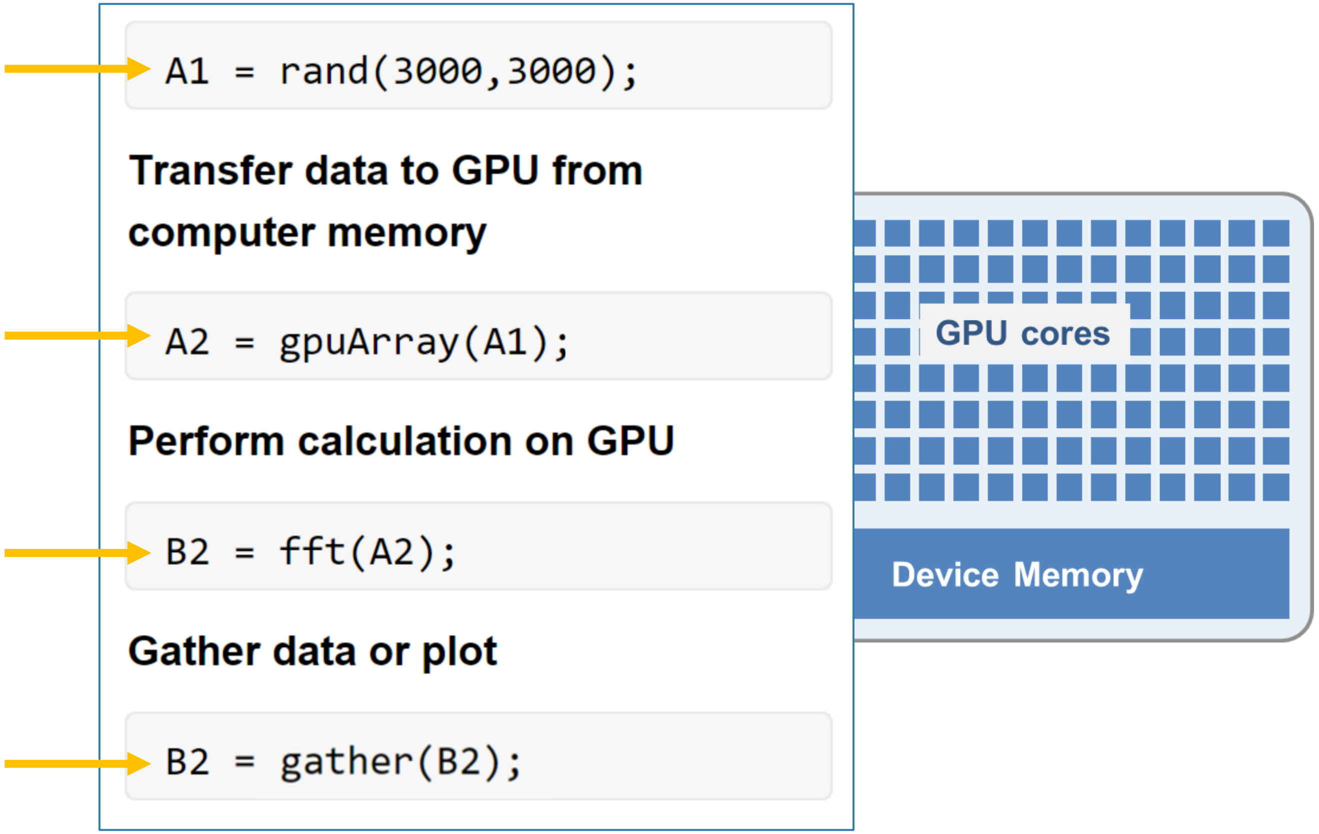
Leverage NVIDIA GPUs without learning CUDA



MATLAB
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



```
A1 = rand(3000,3000);
```

Transfer data to GPU from computer memory

```
A2 = gpuArray(A1);
```

Perform calculation on GPU

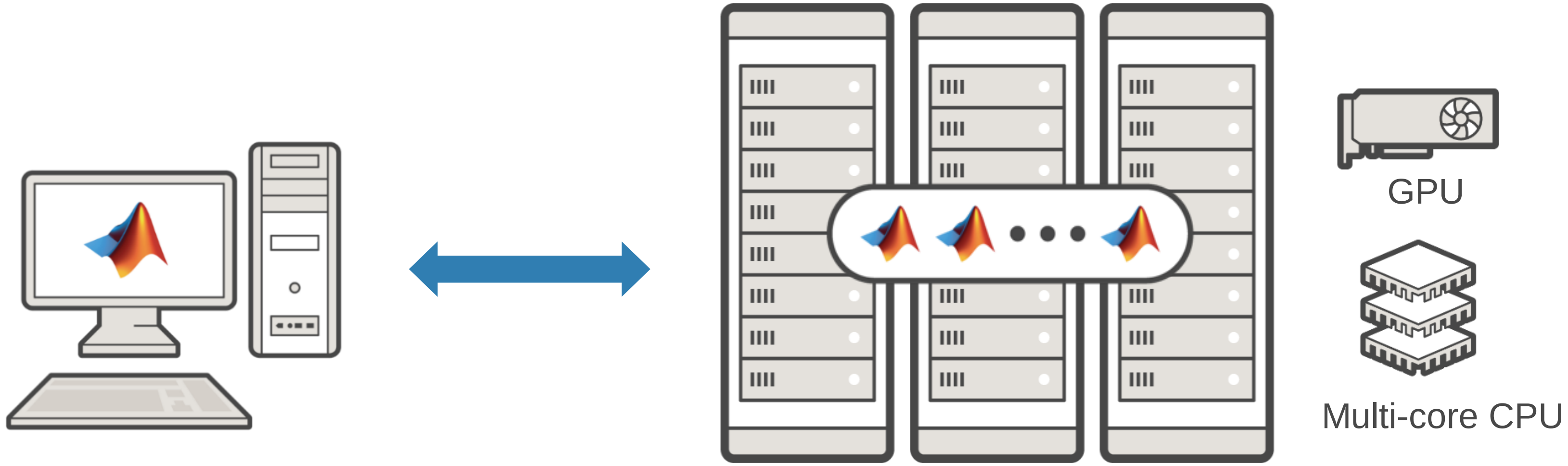
```
B2 = fft(A2);
```

Gather data or plot

```
B2 = gather(B2);
```

MATLAB GPU computing

Parallel computing on your desktop, clusters, and clouds



GPU

Multi-core CPU

MATLAB
Parallel Computing Toolbox

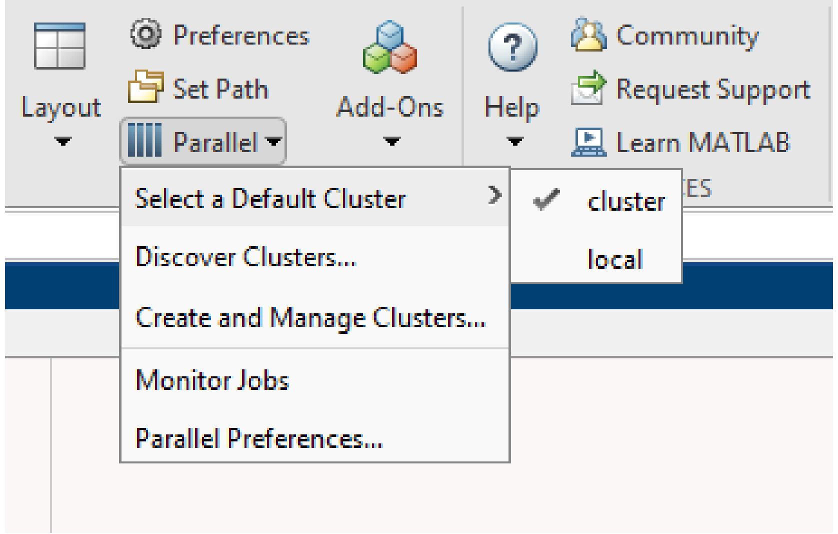
MATLAB Parallel Server

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

Scale to clusters and clouds

With MATLAB Parallel Server, you can…

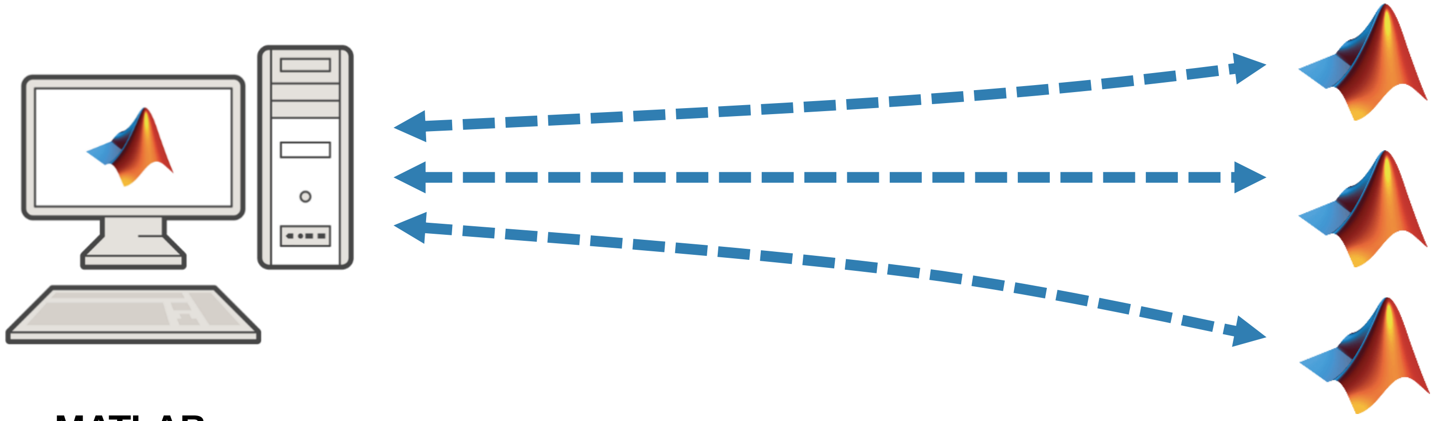
- Change hardware with minimal code change
- Submit to on-premise or cloud clusters
- Support cross-platform submission
  - Windows client to Linux cluster



Interactive parallel computing

Leverage cluster resources in MATLAB

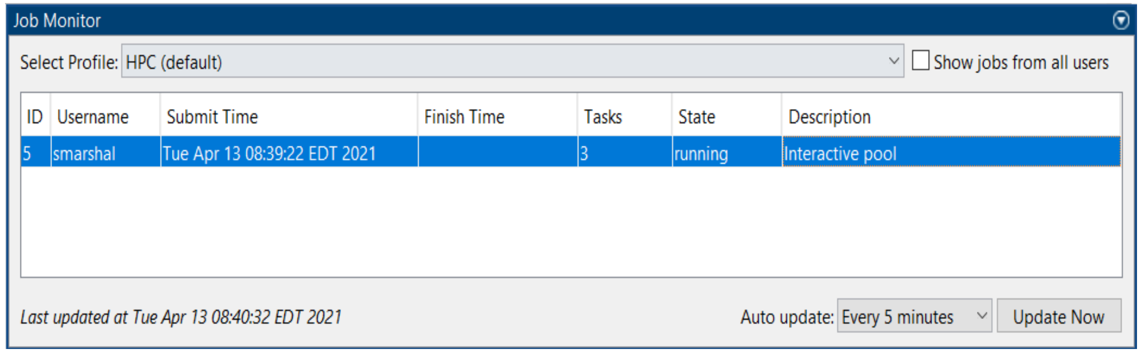
```
>> parpool('cluster', 3);
>> myscript
```



MATLAB
Parallel Computing Toolbox

myscript.m:

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



Job Monitor

Select Profile: HPC (default)

□ Show jobs from all users

ID	Username	Submit Time	Finish Time	Tasks	State	Description
5	smarshal	Tue Apr 13 08:39:22 EDT 2021		3	running	Interactive pool

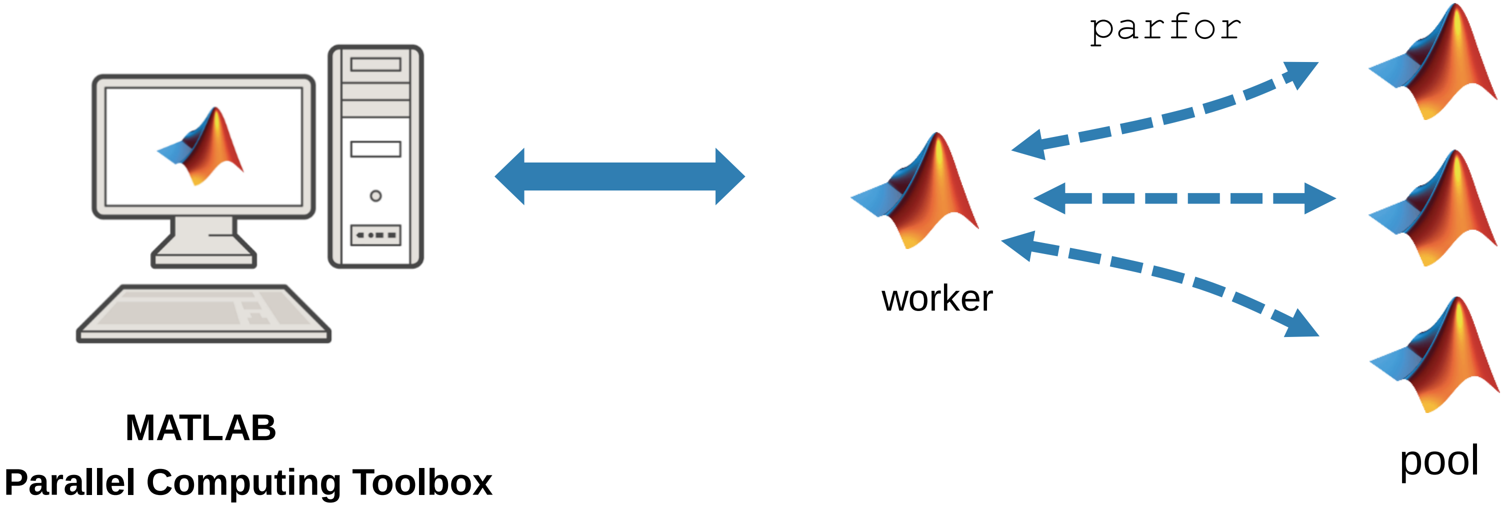
Last updated at Tue Apr 13 08:40:32 EDT 2021

Auto update: Every 5 minutes

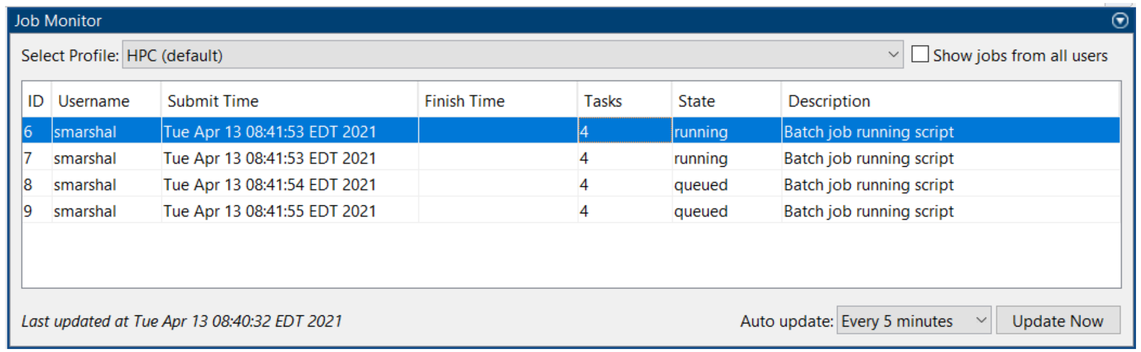
`batch` simplifies offloading computations

Submit MATLAB jobs to the cluster

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



```
>> 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 ---
```



Select Profile: HPC (default) □ Show jobs from all users

ID	Username	Submit Time	Finish Time	Tasks	State	Description
6	smarshal	Tue Apr 13 08:41:53 EDT 2021		4	running	Batch job running script
7	smarshal	Tue Apr 13 08:41:53 EDT 2021		4	running	Batch job running script
8	smarshal	Tue Apr 13 08:41:54 EDT 2021		4	queued	Batch job running script
9	smarshal	Tue Apr 13 08:41:55 EDT 2021		4	queued	Batch job running script

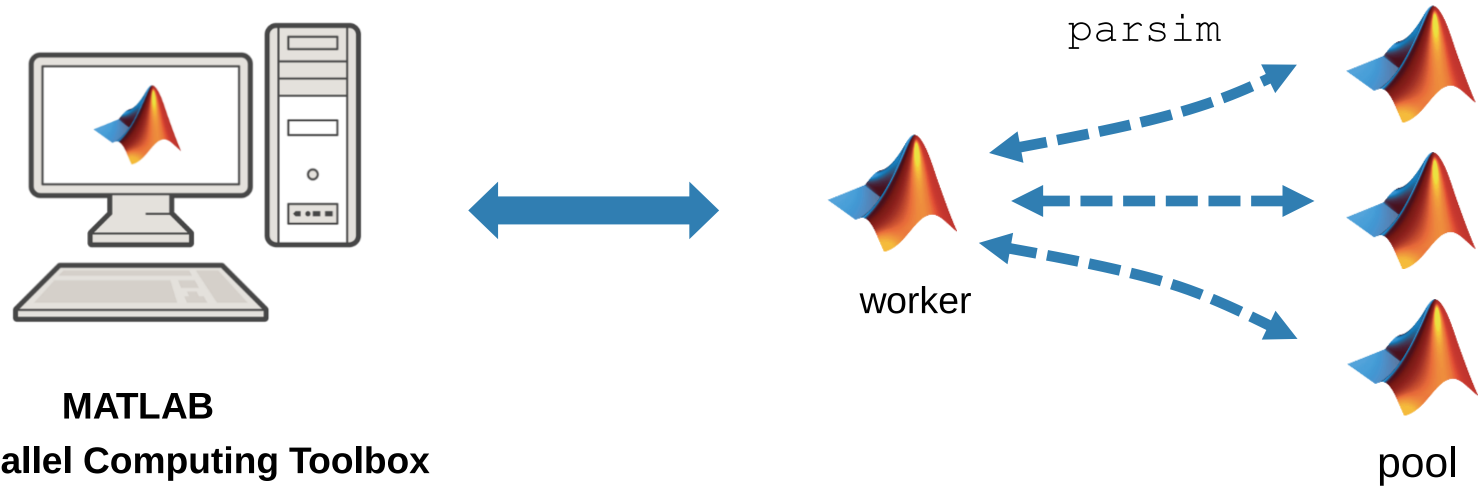
Last updated at Tue Apr 13 08:40:32 EDT 2021

Auto update: Every 5 minutes

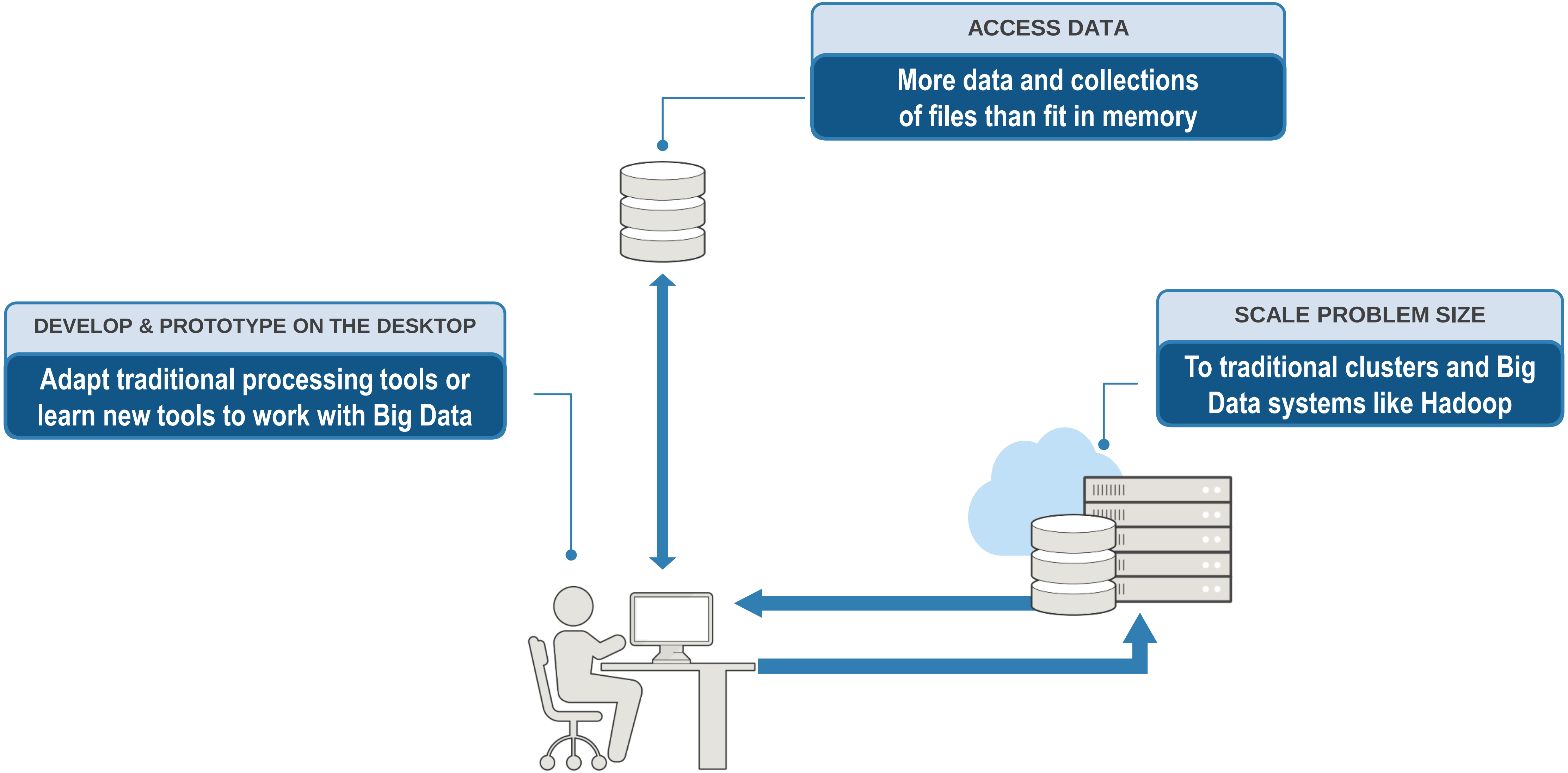
`batch` simplifies offloading simulations

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

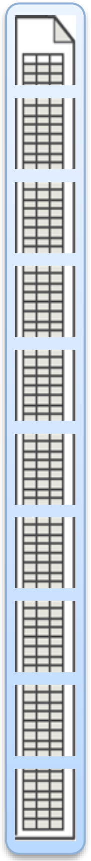
Adapt traditional processing tools or learn new tools to work with Big Data

SCALE PROBLEM SIZE

To traditional clusters and Big Data systems like Hadoop

`tall` arrays

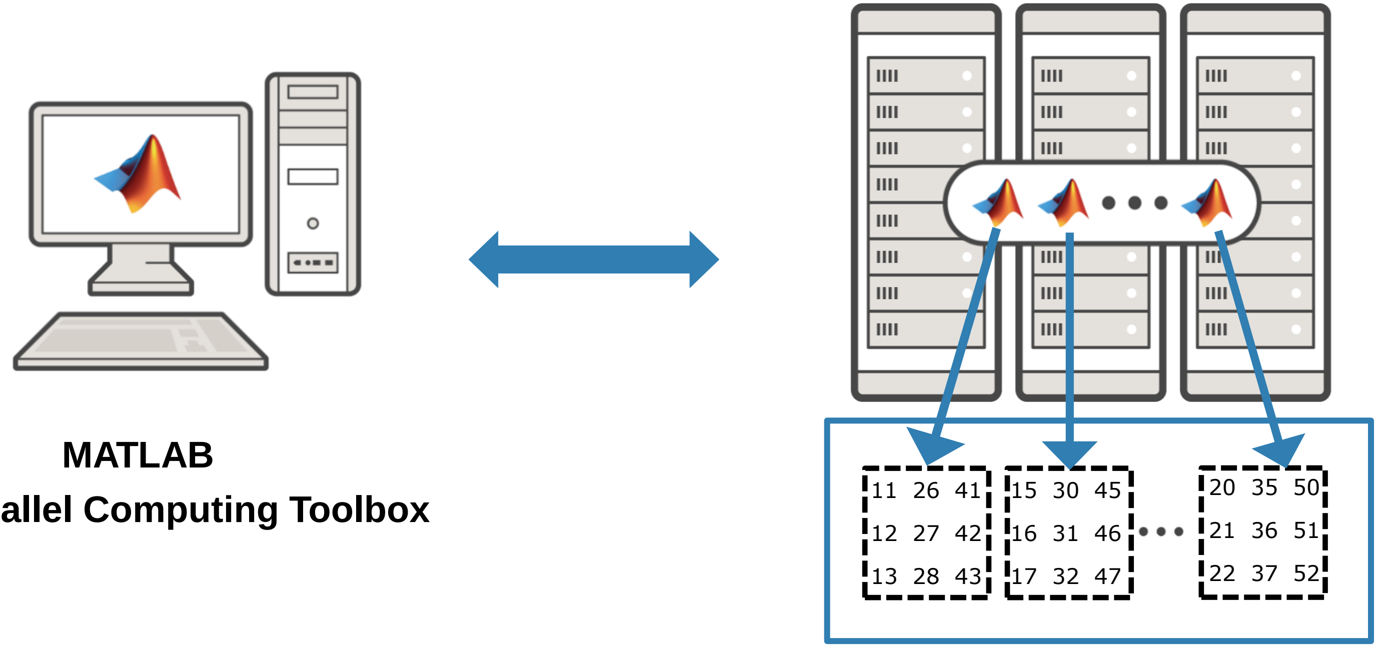
- New data type designed for data that doesn’t fit into memory
- Lots of observations (hence “tall”)
- Looks like a normal MATLAB array
  - Supports numeric types, tables, datetimes, strings, etc.
  - Supports several hundred functions for basic math, stats, indexing, etc.
  - Statistics and Machine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



Working with tall arrays

`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



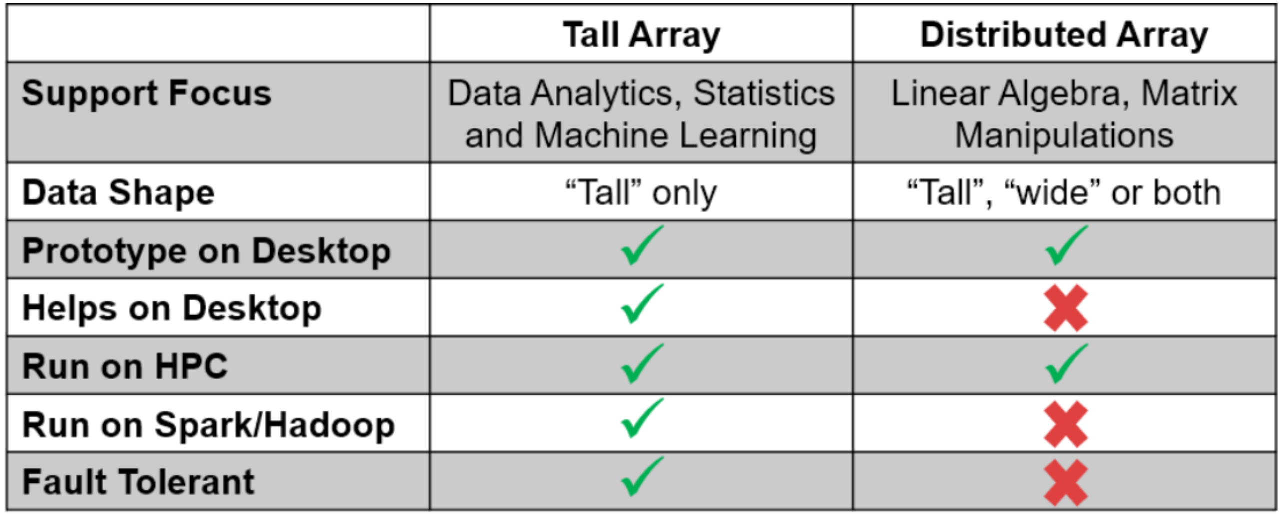
MATLAB
Parallel Computing Toolbox

11 26 41 | 15 30 45 | … | 20 35 50
12 27 42 | 16 31 46 | … | 21 36 51
13 28 43 | 17 32 47 | … | 22 37 52

MATLAB Parallel Server

`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	✓	✗

Resources

- MATLAB Documentation
  - MATLAB → Advanced Software Development → Performance and Memory
  - Parallel Computing Toolbox

- Parallel and GPU Computing Tutorials
  - https://www.mathworks.com/videos/series/parallel-and-gpu-computing-tutorials-97719.html

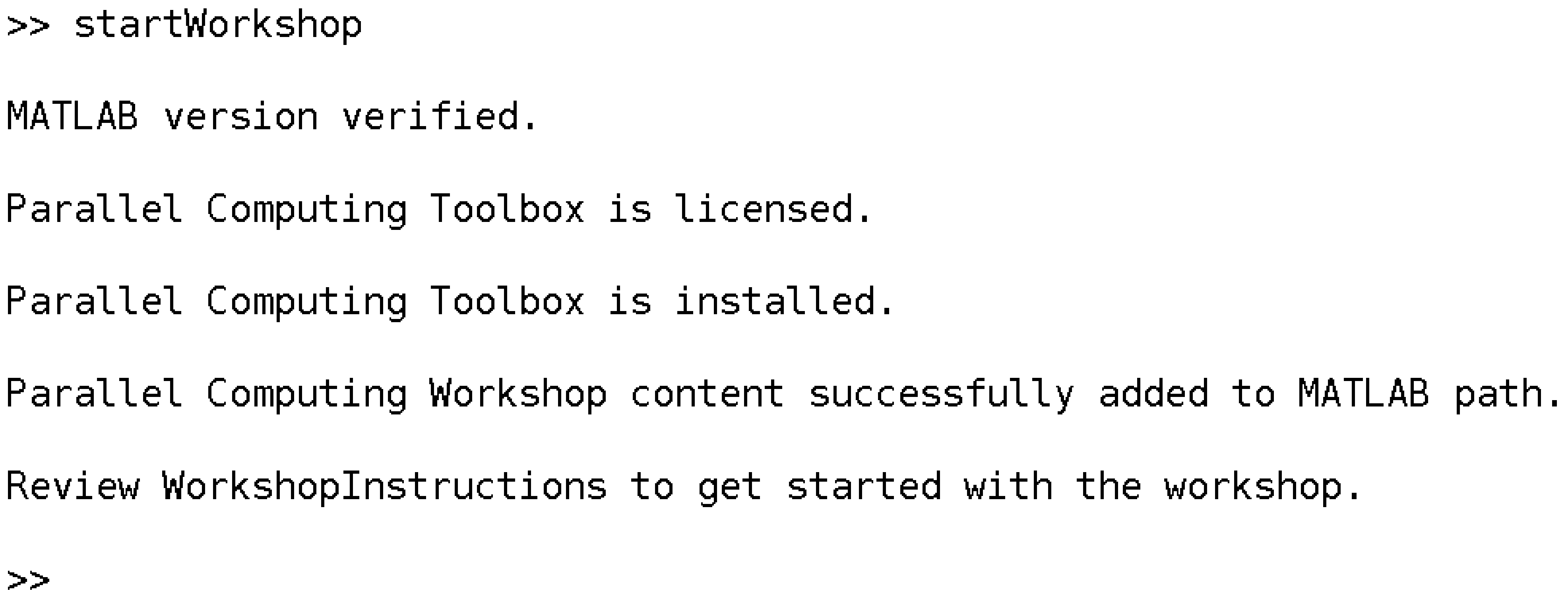
- Parallel Computing with MATLAB
  - https://www.mathworks.com/solutions/parallel-computing.html

Download Instructions

- https://drive.matlab.com/sharing/8bd444df-1344-429e-aa71-1da85bf81870
  - Click on **Add to my Files**
  - Click **Copy Folder**
  - Log into MATLAB Drive with MathWorks Account

- https://www.mathworks.com/licensecenter/classroom/PC_3507600
  - Enter MathWorks email address
  - Click **Next**
  - Click **Access MATLAB Online** (maybe prompted to sign-in again)
  - In Current Folder, double click on **Parallel Computing Workshop**
  - Right click on **startWorkshop**, select **Run**

Start Workshop



```
>> startWorkshop
MATLAB version verified.
Parallel Computing Toolbox is licensed.
Parallel Computing Toolbox is installed.
Parallel Computing Workshop content successfully added to MATLAB path.
Review WorkshopInstructions to get started with the workshop.
>>
```

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