High Performance Computing with MATLAB

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MathWorks China

Outline

- Before we go parallel: Code optimization for better performance
- How to write and run parallel MATLAB code on your local machine or a cluster
- How to run MATLAB code on GPUs to accelerate your computations
- Use big data processing methods to handle large datasets
- Learning Resources

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! 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
```

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

Elapsed time is 0.075824 seconds.

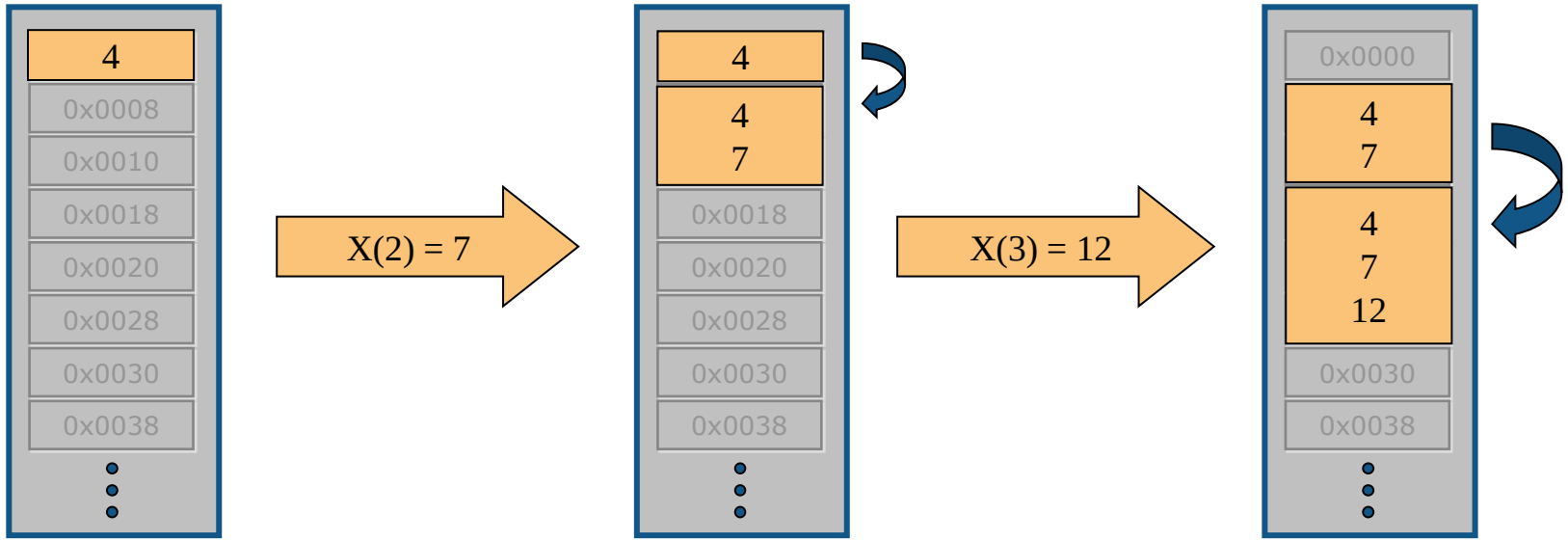
```
1  tic
2  x = zeros(1,1e6);
3  for k = 2:1e6
4      x(k) = x(k-1) + 1;
5  end
6  toc
```

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

Elapsed time is 0.013109 seconds.

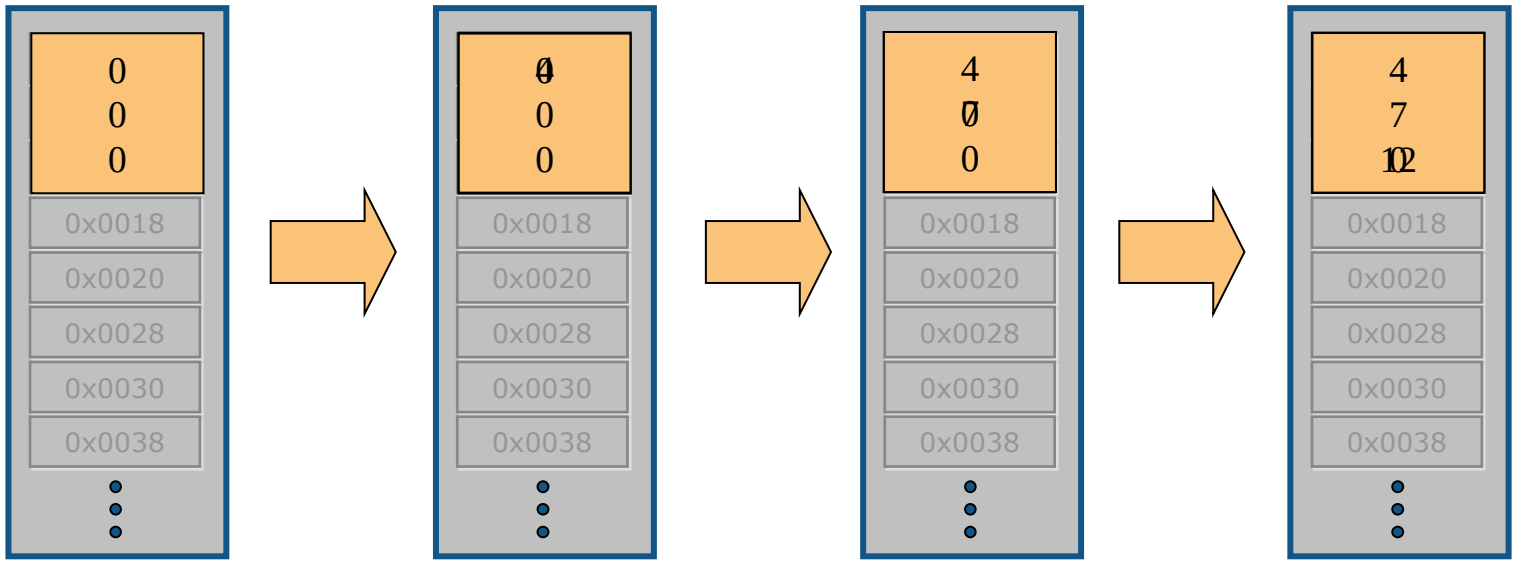
Effect of Not Preallocating Memory

```
x(1) = 4
x(2) = 7
x(3) = 12
```



Benefit of Preallocation

```
x = zeros(3,1)
x(1) = 4
x(2) = 7
x(3) = 12
```



Demo: Preallocation

```
tic
x = 0;
for k = 2:1000000
   x(k) = x(k-1) + 5;
end
toc

Elapsed time is 0.301528 seconds.
```

```
tic
x = zeros(1, 1000000);
for k = 2:1000000
   x(k) = x(k-1) + 5;
end
toc

Elapsed time is 0.011938 seconds.
```

Vectorization

Vectorizing a scalar loop

```
i = 0;
for t = 0:.01:10
    i = i + 1;
    y(i) = sin(t);
end
```



```
t = 0:.01:10;
y = sin(t);
```

Array operations: leveraging operators and implicit expansion

```
mA = mean(A);
B = zeros(size(A));
for n = 1:size(A,2)
    B(:,n) = A(:,n) - mA(n);
end
```



```
devA = A - mean(A)
```

Logical array operations: logical indexing

```
for c = 1:N
    for r = 1:N
        if A(r,c) > myRef
            B(r,c) = A(r,c);
        end
    end
end
```

```
B(A > myRef) = A(A > myRef);
```

A(*logical*)

Matrix operations, sorting, etc.

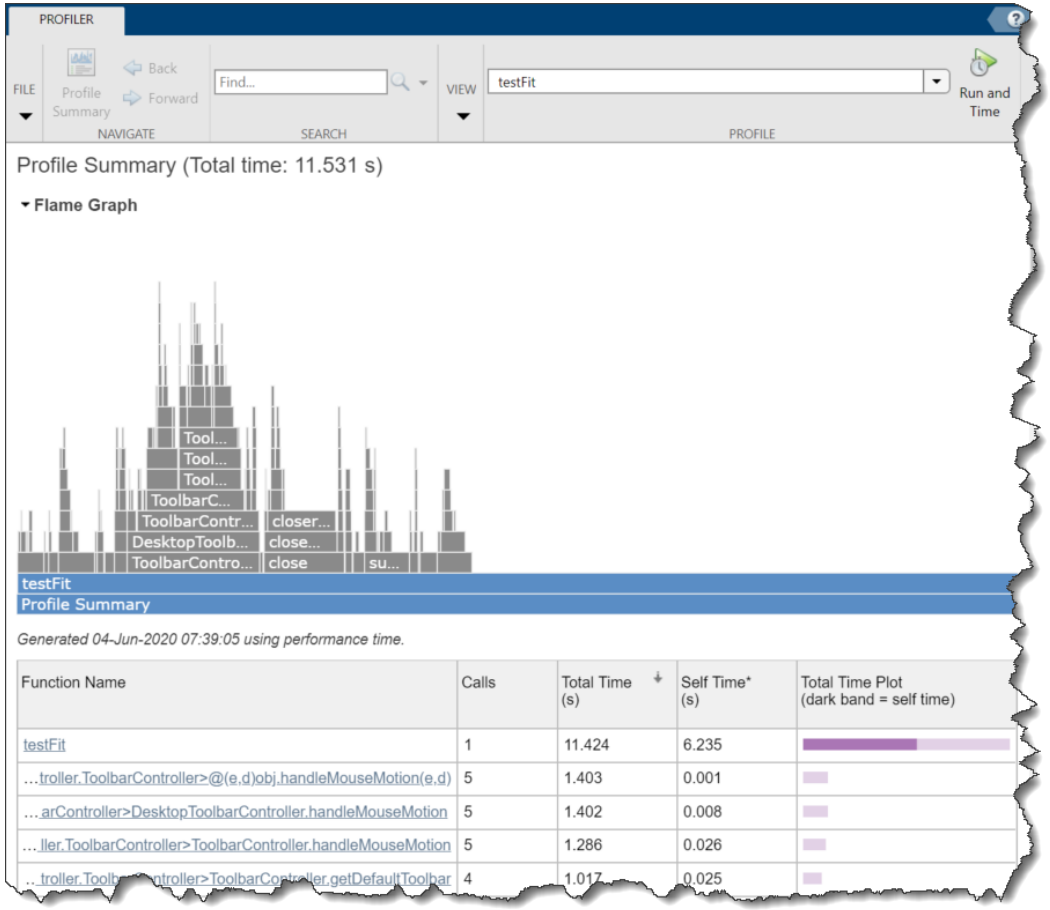
Functions Commonly Used in Vectorization

Function	Descrip
all	Determ
any	Determ
cumsum	Cumula
diff	Differer
find	Find inc
ind2sub	Subscri
ipermute	Inverse
logical	Conver
meshgrid	Rectan
ndgrid	Rectan
permute	Rearrar
prod	Produc
repmat	Repeat
reshape	Reshap
shiftdim	Shift di
sort	Sort arr
squeeze	Remov
sub2ind	Conver
sum	Sum of

https://www.mathworks.com/help/releases/R2023a/matlab/matlab_prog/vectorization.html

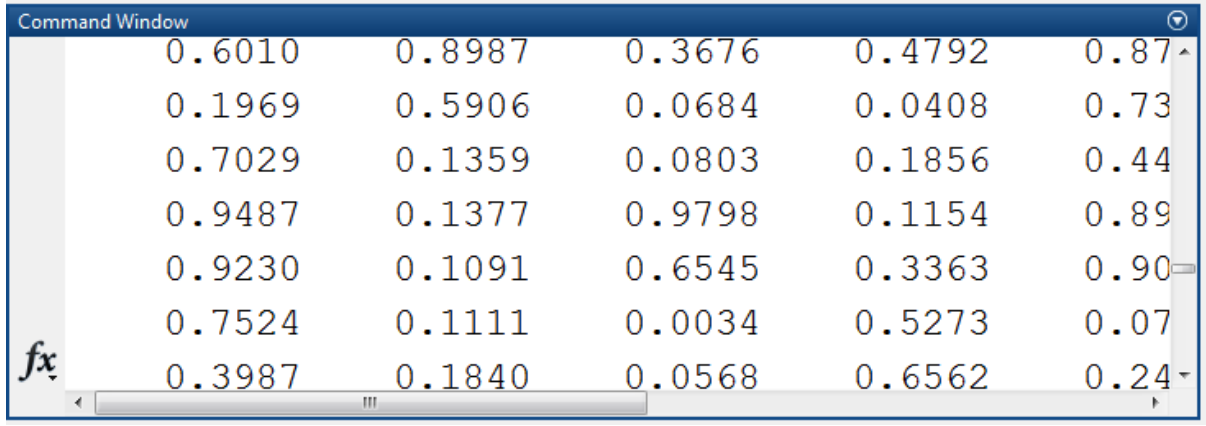
Profiler

- Total number of function calls
- Time per function call
- Self time in a function call
- Statement coverage of code



Best Practices

- Minimize file I/O
- Reuse existing graphics components
- Avoid printing to Command Window



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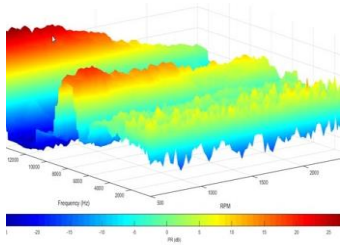
Practical application of parallel computing

- Why parallel computing?
  - Need faster insight to bring competitive products to market quickly
  - Computing infrastructure is broadly available (multicore desktops, GPUs, clusters)

- Why parallel computing with MATLAB?
  - Leverage computational power of more hardware
  - Accelerate workflows with minimal to no code changes to your original code
  - Focus on your engineering and research, not the computation

Results for scaling to more CPU cores and GPUs



Automotive Test Analysis
Validation time sped up 2X
Development time reduced 4 months

Discrete-Event Model of Fleet Performance
Simulation time sped up 20X
Simulation time reduced from months to hours

Heart Transplant Study
Process time sped up 6X
4-week process reduced to 5 days

Calculating Derived Market Data
Updates sped up 8X
Updates reduced from weeks to days

User stories

FICC Department of China Galaxy Securities Valuates Financial Assets and Builds Training and Hedging Strategies

Challenge

Perform large amounts of complicated quantitative analysis under time pressure

Solution

Use MATLAB and its finance toolboxes to model and develop investment strategies

Results

- Run times reduced to a couple of minutes
- Quality of work improved
- Work efficiency increased

The FICC department of China Galaxy Securities applies MATLAB in their investment strategies.

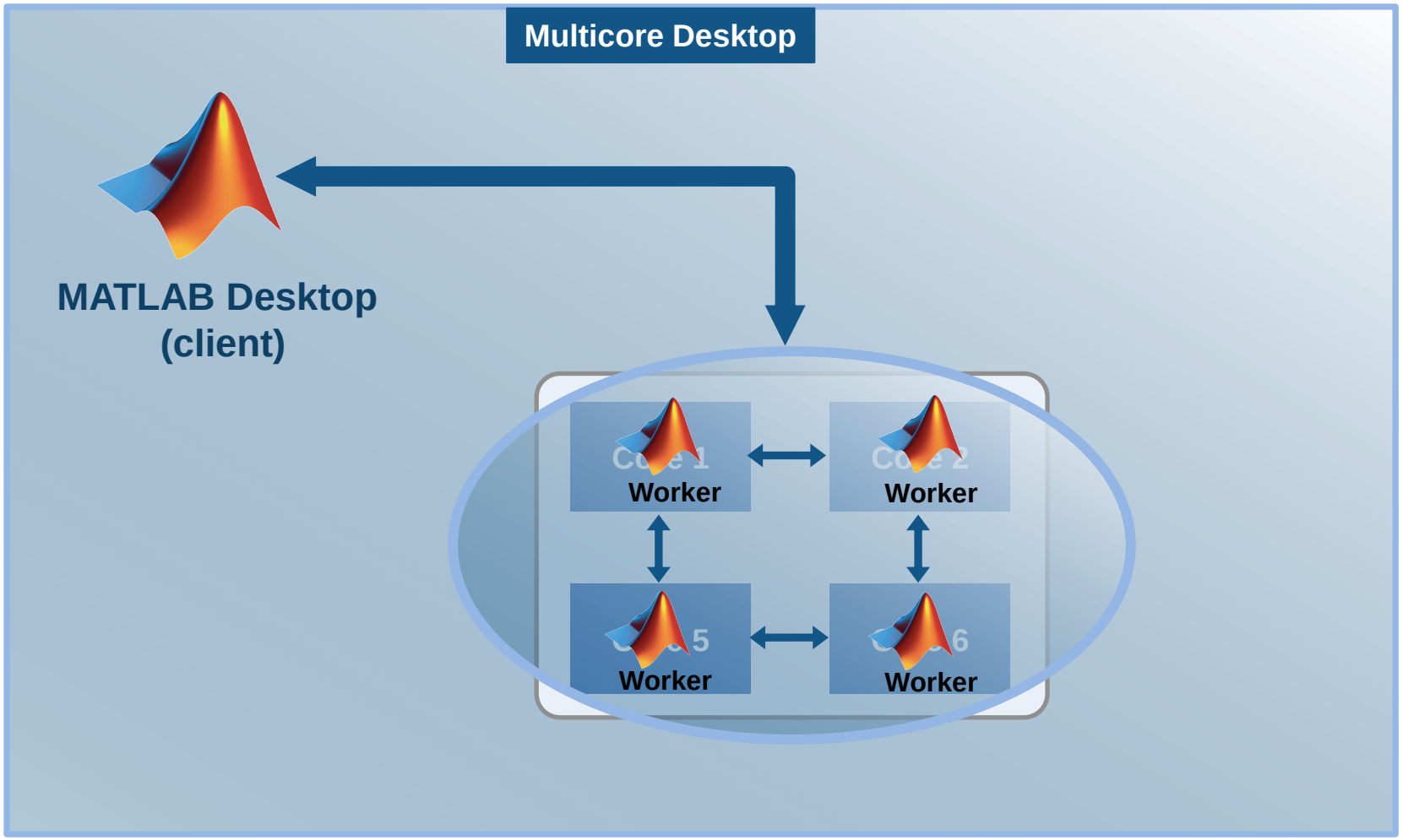
"Investments in fixed income, currency, and commodities require large amounts of quantitative analysis. MATLAB supports us with highly efficient development tools for the valuation of financial instruments, statistical analysis of financial data, and the building and backtesting of quantitative strategies."

- Xian Xingchi, China Galaxy Securities

Link to user story

Parallel Computing Paradigm

Multicore Desktops



MATLAB multicore

Accelerating MATLAB Applications

Parallel-enabled toolboxes

```
('UseParallel', true)
```

Common programming constructs

Advanced programming constructs

Enable parallel computing support by setting a flag or preference

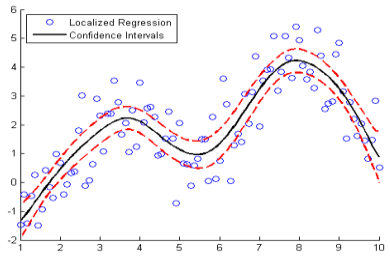
Automatic parallel support *(MATLAB)*

Image Processing

Batch Image Processor, Block Processing, GPU-enabled functions

Statistics and Machine Learning

Resampling Methods, k-Means clustering, GPU-enabled functions

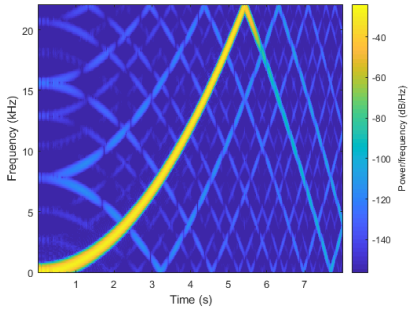


Deep Learning

Deep Learning, Neural Network training and simulation

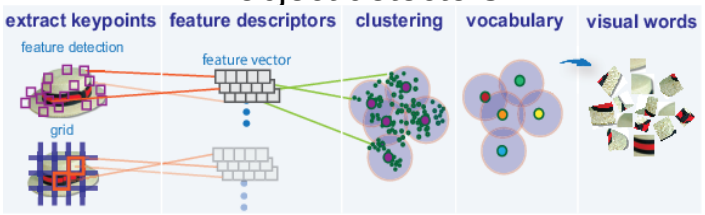
Signal Processing and Communications

GPU-enabled FFT filtering, cross correlation, BER simulations



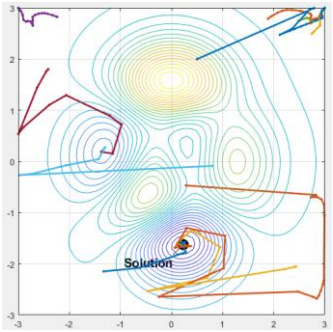
Computer Vision

Bag-of-words workflow, object detectors



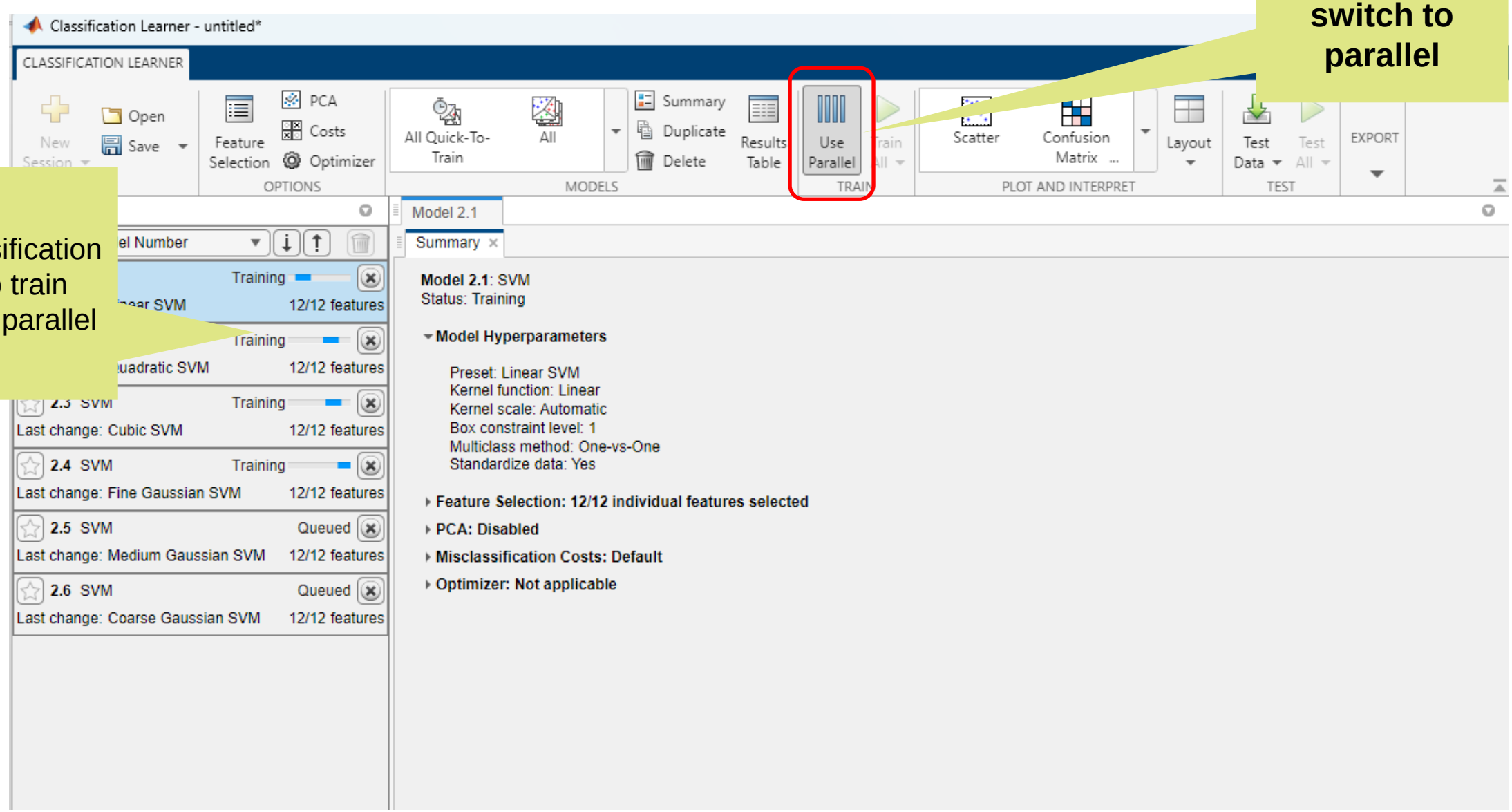
Optimization and Global Optimization

Estimation of gradients, parallel search



[Additional automatic parallel support]

Classification Learner



Use Classification Learner to train models in parallel

Click here to switch to parallel

Scaling MATLAB applications and Simulink simulations

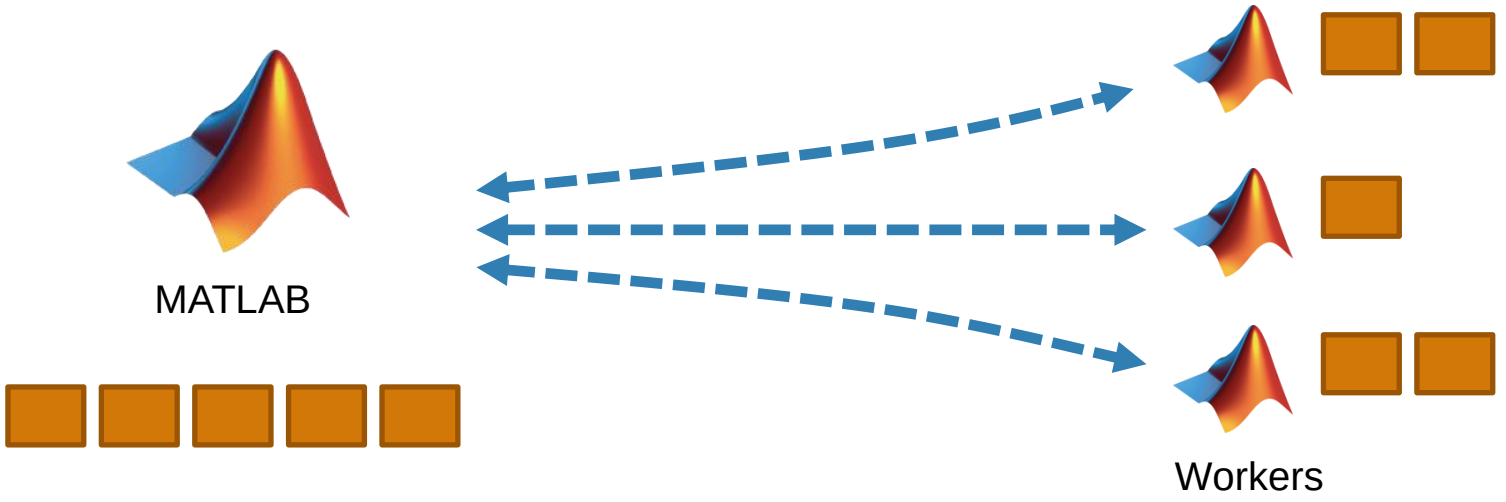
Automatic parallel support in toolboxes

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

Advanced programming constructs

Run independent iterations in parallel using `parfor`

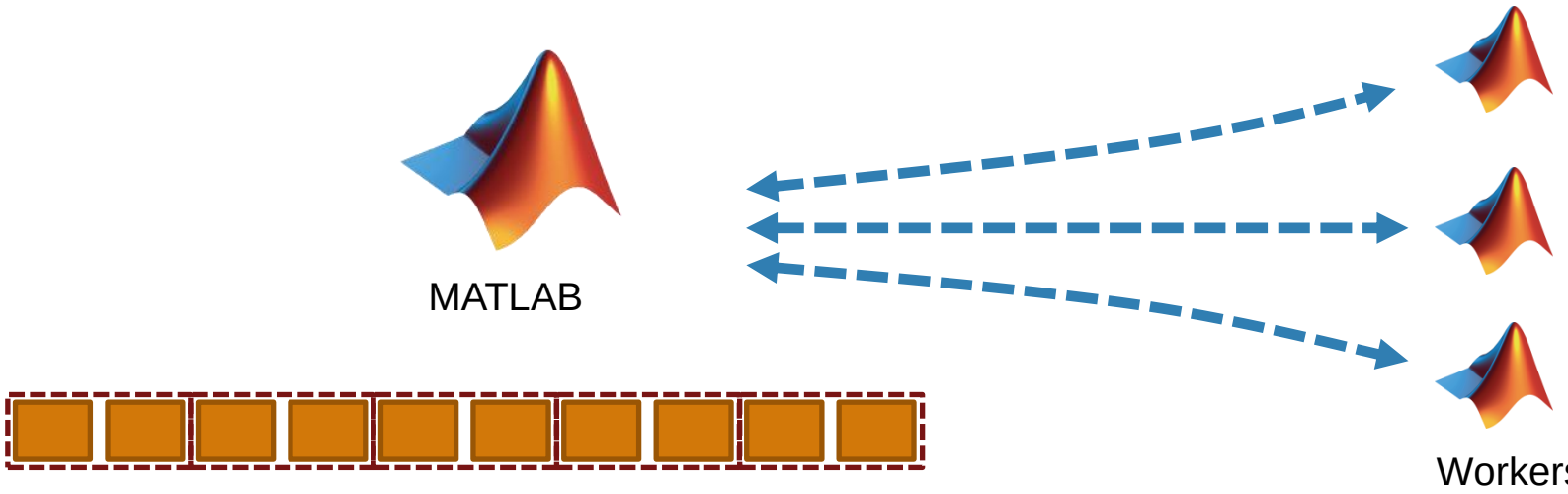
Use cases: Parameter sweeps and Monte Carlo simulations




```
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)
```

Parallelize for loops with independent iterations




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

Demo: Compute the largest eigenvalue (serial)

```
>> edit ex_serial
```

```
function a = ex_serial(M, N)
% EX_SERIAL performs N trials of
%  computing the largest eigenvalue
% for an M-by-M random matrix

a = zeros(N,1);
for I = 1:N
    a(I) = max(eig(rand(M)));
end
```

Demo: Compute the largest eigenvalue (parallel)

```
>> edit ex_parallel
```

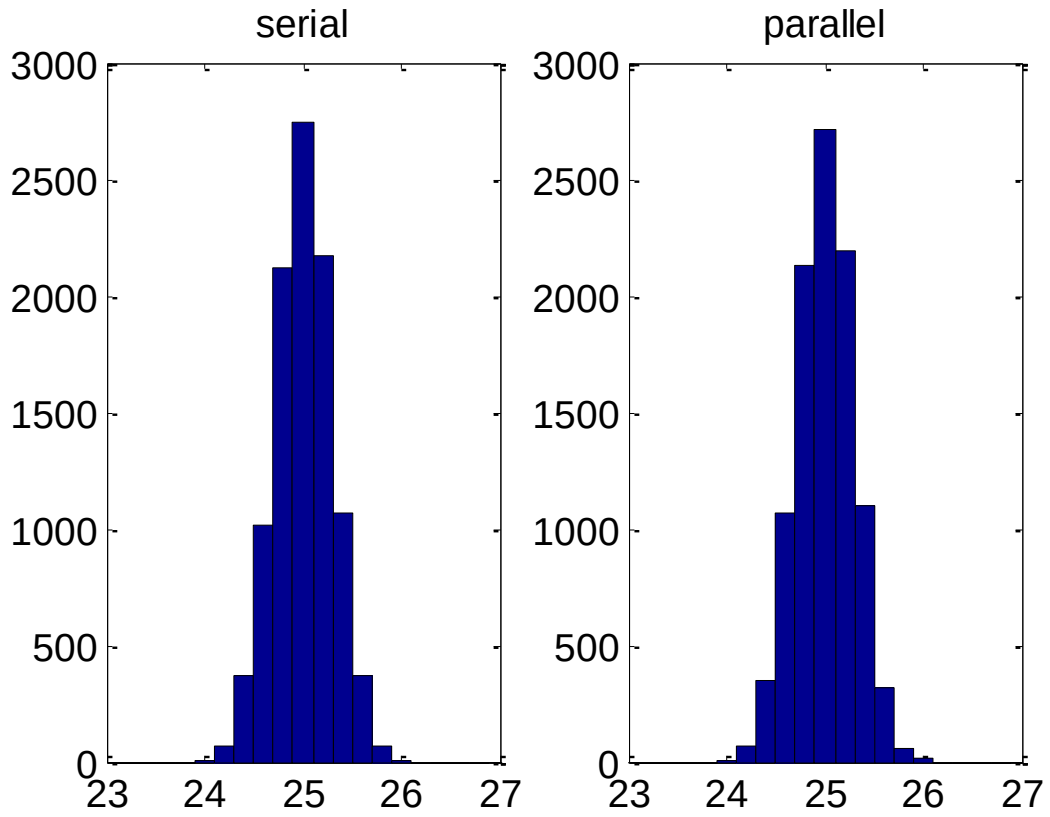
```
function a = ex_parallel(M, N)
% EX_PARALLEL performs N trials of
%  computing the largest eigenvalue
% for an M-by-M random matrix

a = zeros(N,1);
parfor I = 1:N
    a(I) = max(eig(rand(M)));
end
```

The only modification!

Performance Comparation

```
>> edit ex_compare
>> ex_compare
```

Serial processing time: 8.6s
Parallel processing time: 2.7s



Minor modifications resulted in a significant increase in speed.

`parfor` limitation

Noninteger loop variable

```
parfor x = 0:0.1:1
```

Nested parallel loops 

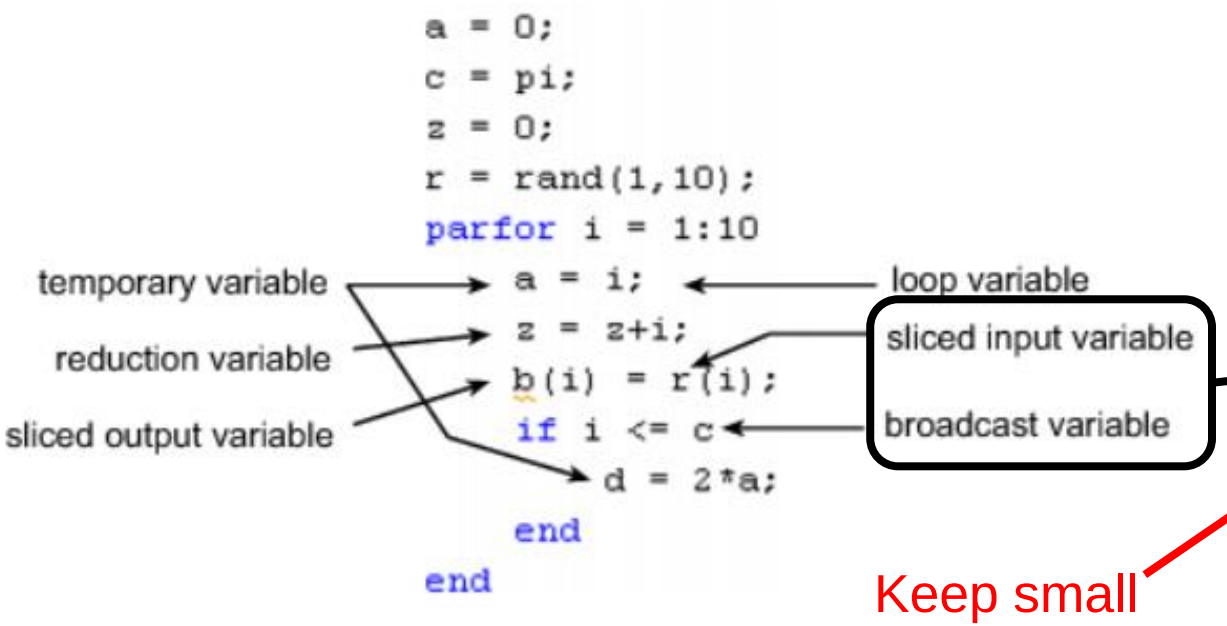
```
    parfor y = 2:10

        A(y) = A(y-1) + ...
```

```
    end
```

Dependent loop body

```
end
```

Optimizing `parfor`



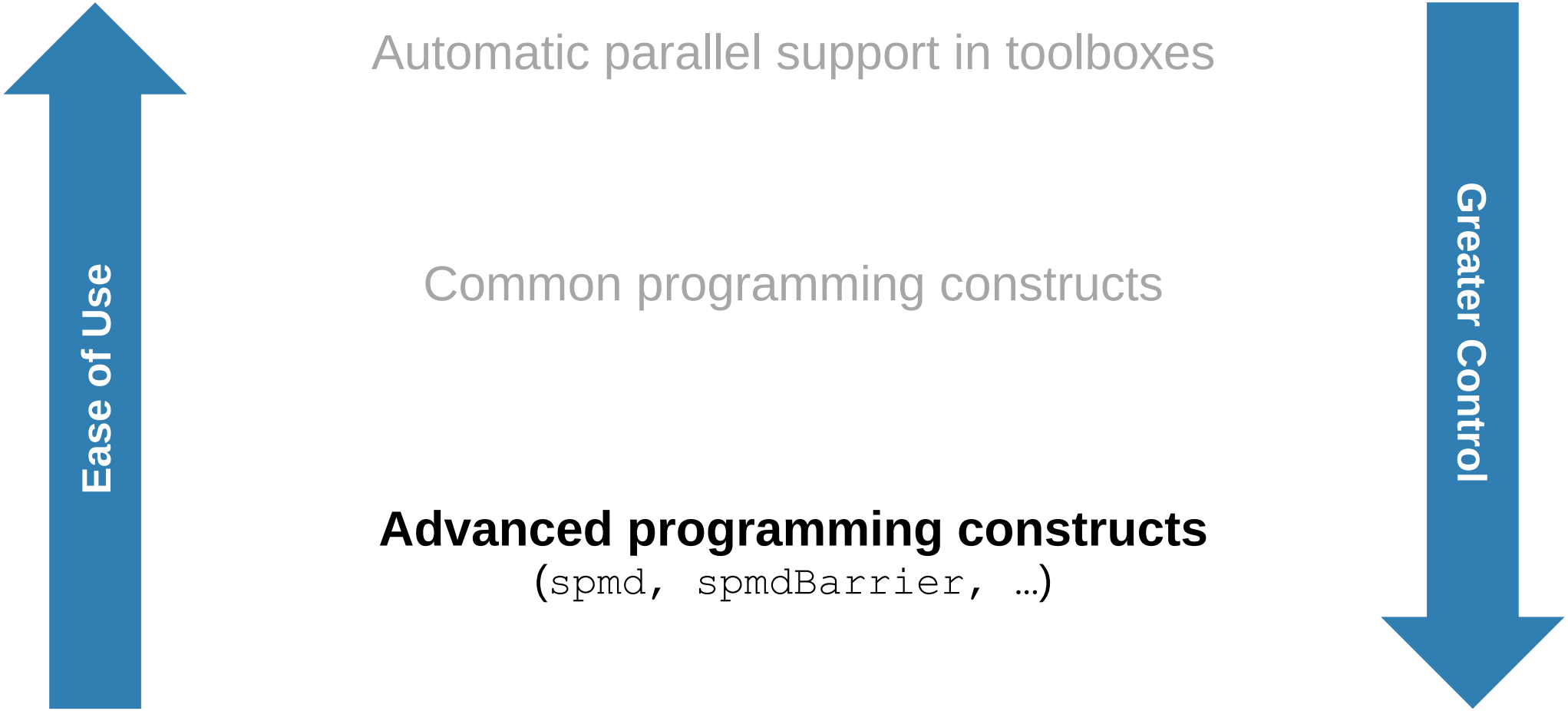
Use more

Keep small

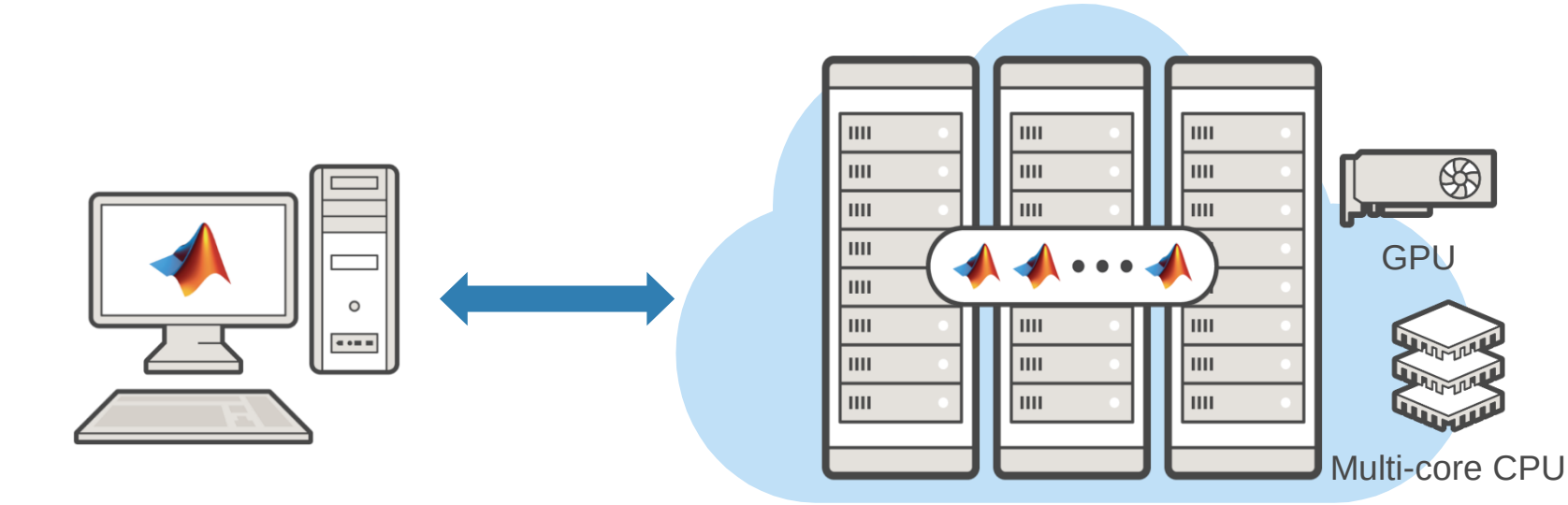
Type	Category
sliced input	input
broadcast	input
reduction	output
sliced output	output
loop	only exist on worker
temporary	only exist on worker

Troubleshooting variables in parfor-loops

Scaling MATLAB applications and Simulink simulations



Parallel computing on your desktop, clusters, and clouds

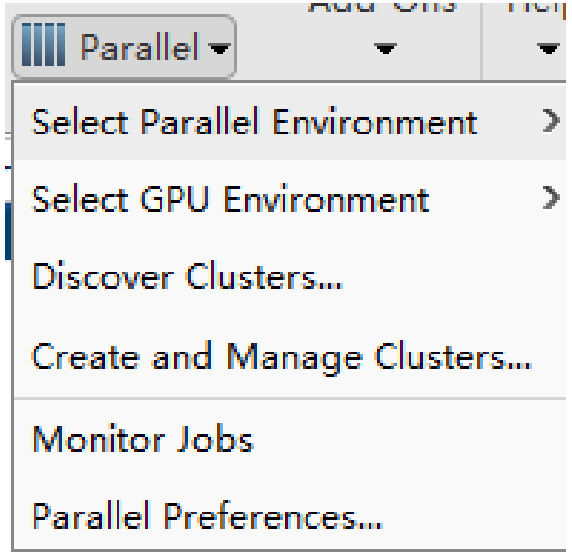


- Prototype and develop on the desktop
- Integrate with your infrastructure
- Access directly through MATLAB

Scale to clusters and clouds

With MATLAB Parallel Server, you can…

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



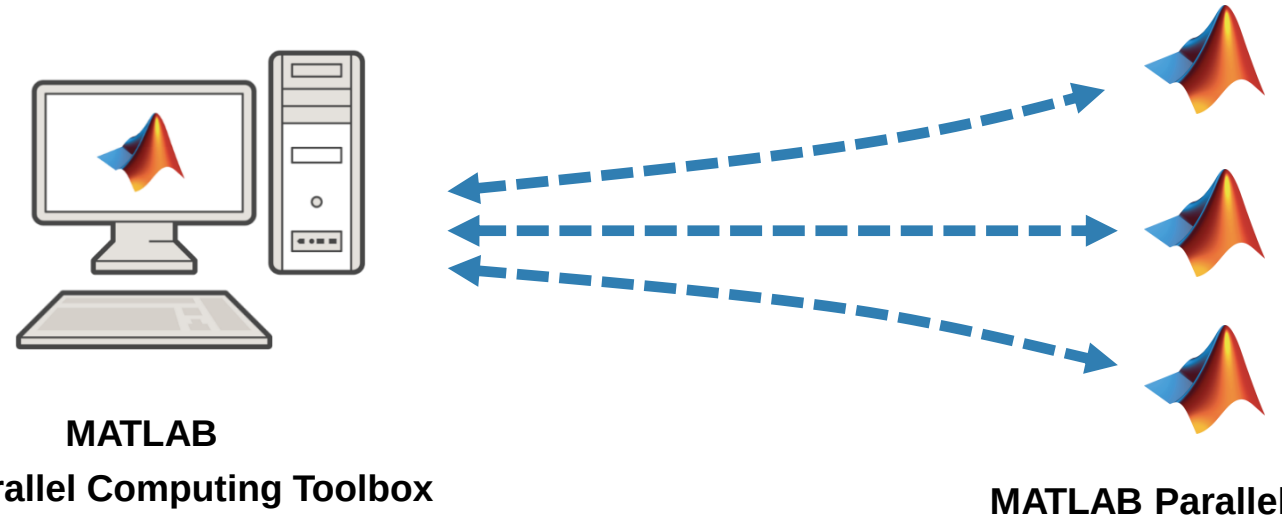
Interactive parallel computing

Leverage cluster resources in MATLAB

```
>> parpool(myCluster,3)
>> myScript
```

myScript.m:

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



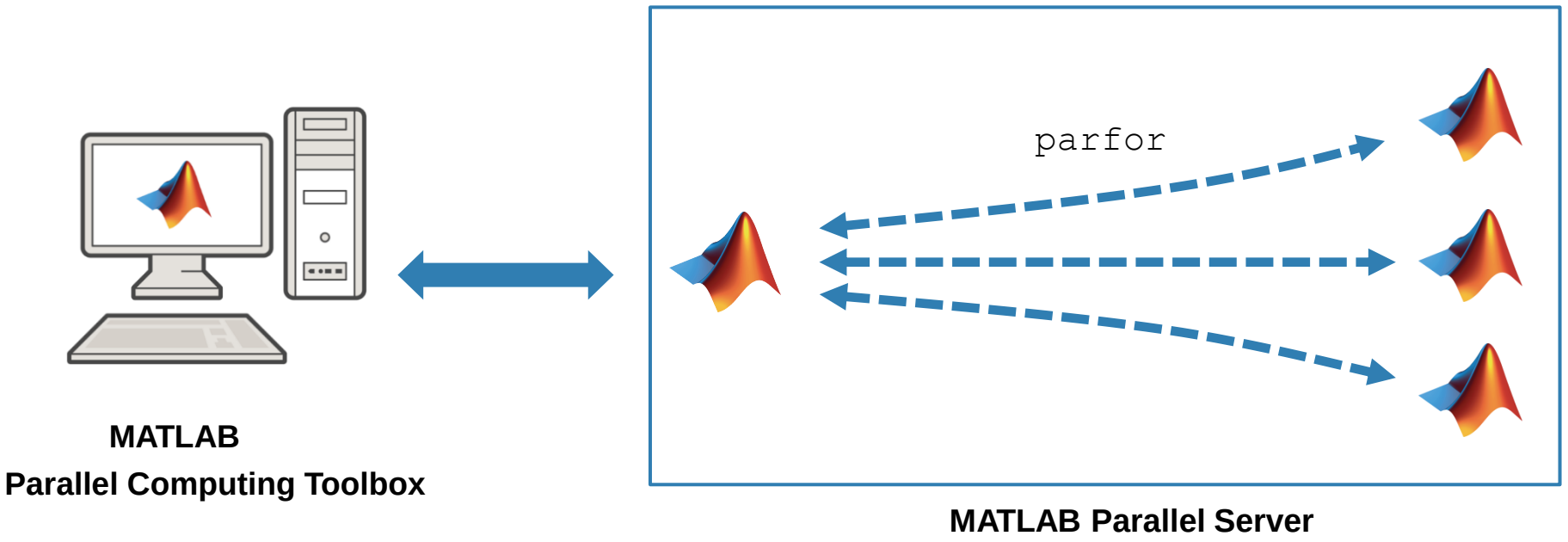
MATLAB
Parallel Computing Toolbox

MATLAB Parallel Server

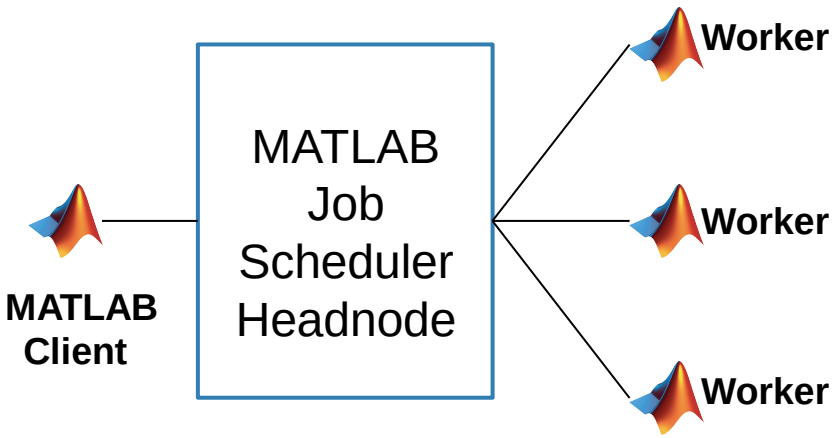
`batch` simplifies offloading computations

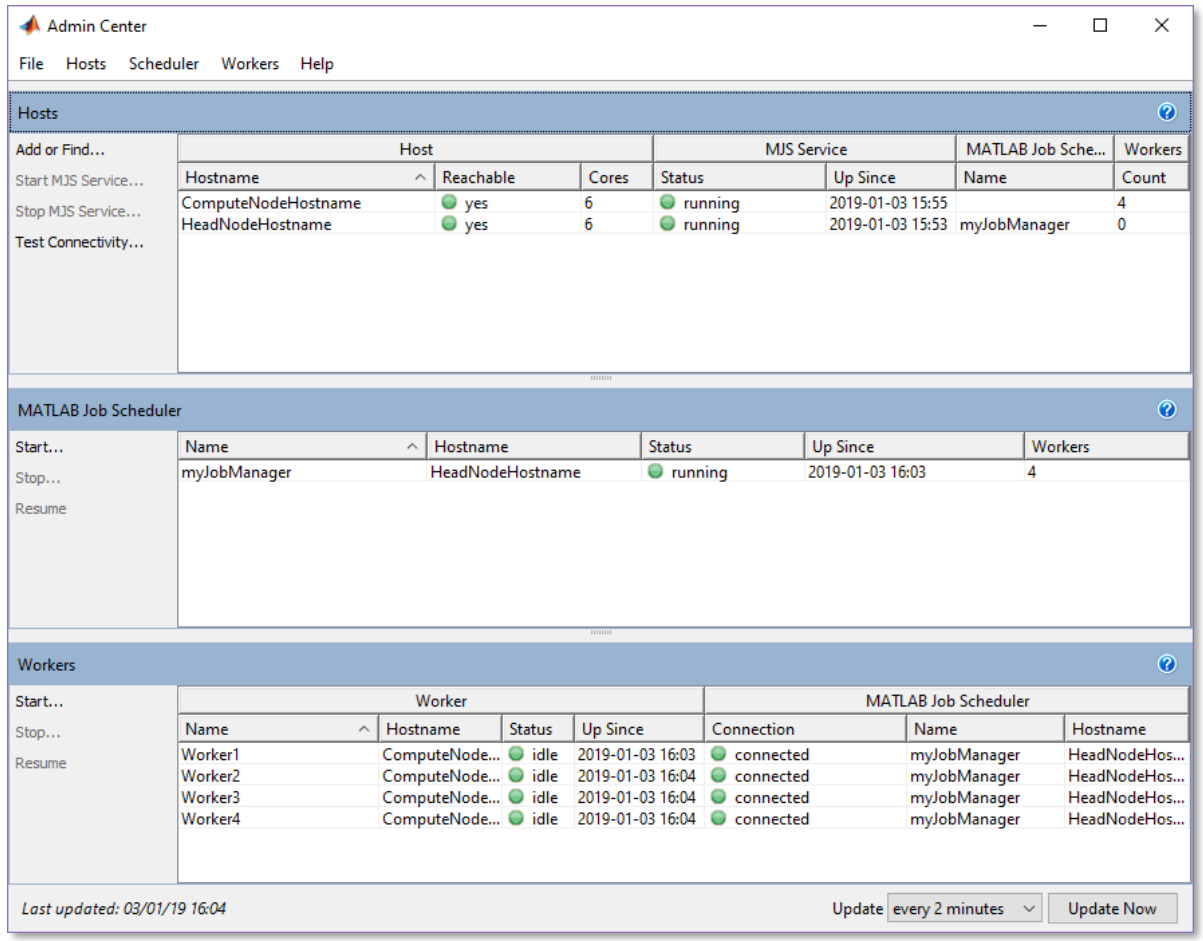
Submit MATLAB jobs to the cluster

```
>> job = batch(myCluster,'myScript','Pool',3)
```



MATLAB Job Scheduler allows you to set up a MATLAB cluster from scratch



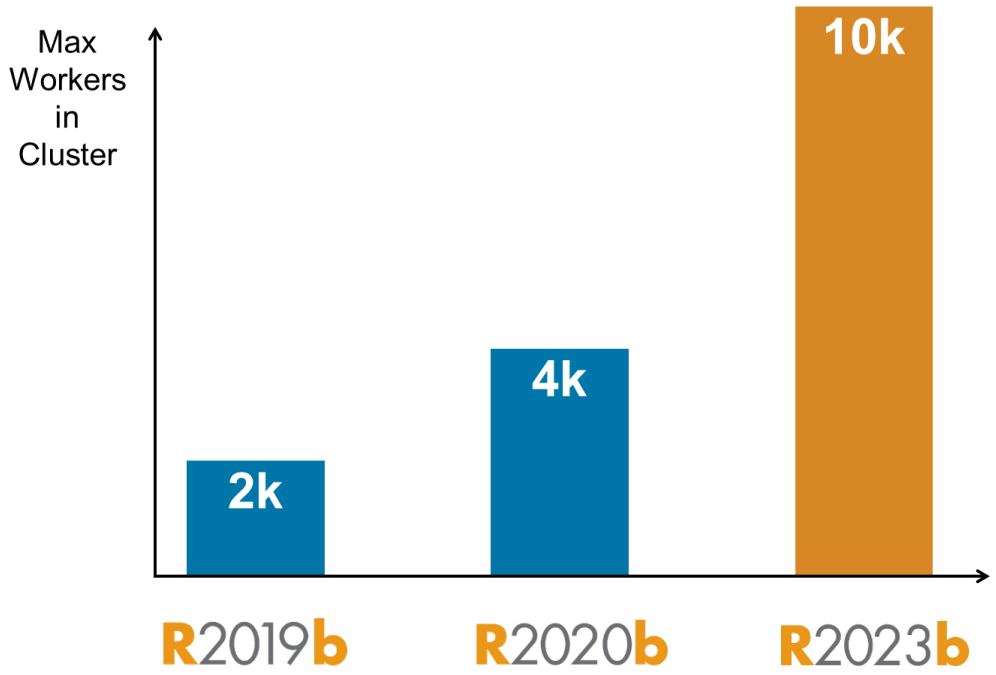


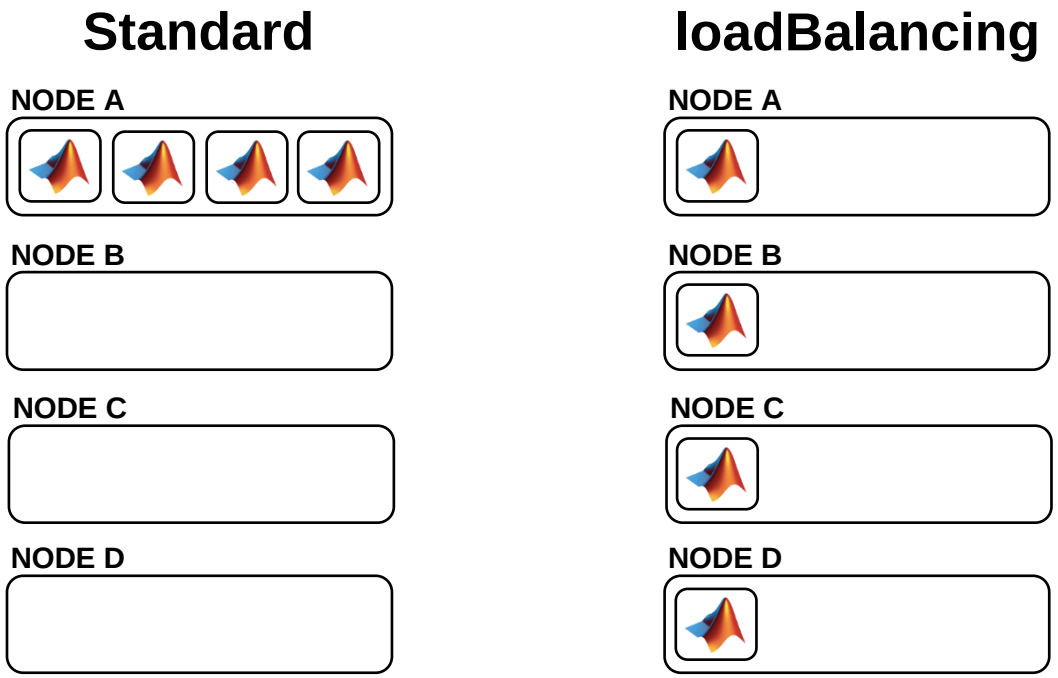
[Additional information]

If you need to install parallel server on your cluster, please contact our dedicated installation support at info@mathworks.cn

Improvements and updates to MATLAB Job Scheduler scalability and scheduling

- MATLAB Job Scheduler supports clusters with up to 10K workers
- Control load-balancing scheduling algorithm on MATLAB Job Scheduler





Support for integration with third-party schedulers

Scheduler	Ready to use options	Customizable via generic scheduler API	Example Plugins available
Slurm	✓	✓	✓
Microsoft® Windows® HPC Server	✓		
Grid Engine family		✓	✓
IBM® Platform LSF	✓	✓	✓
PBS family	✓	✓	✓
HTCondor		✓	✓
Other schedulers		✓	

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Learn More

- Getting started with parallel computing
  - Parallel Computing Toolbox
  - Performance and Memory

- Scaling to the cluster and cloud
  - MATLAB Parallel Server
  - MATLAB Parallel Server on the cloud

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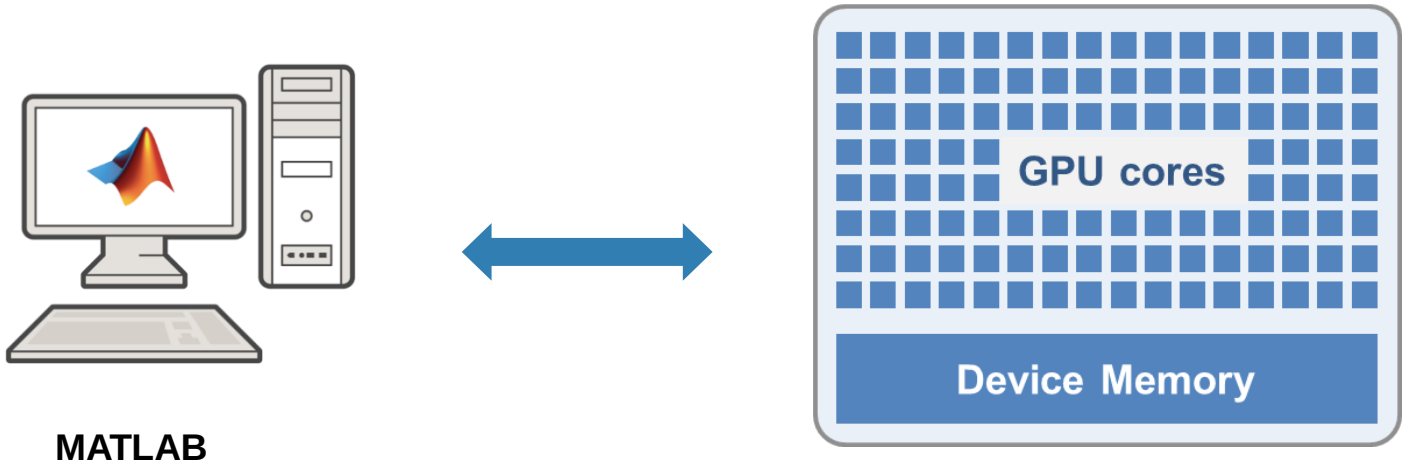
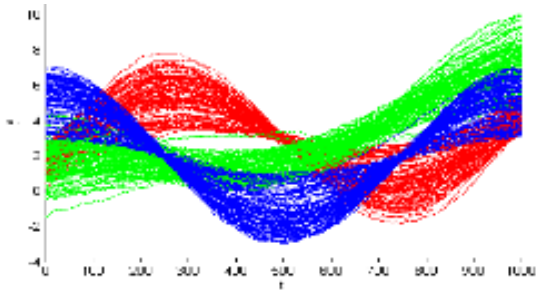
Leverage NVIDIA GPUs without learning CUDA



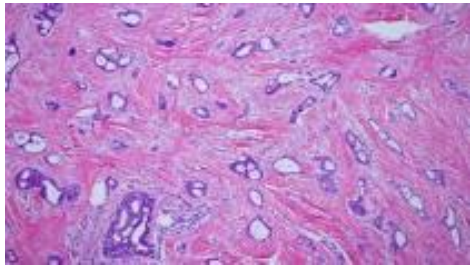
MATLAB

Parallel Computing Toolbox

Results for accelerating with NVIDIA GPUs

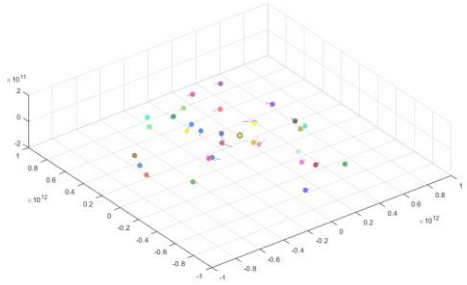


10x speedup
K-means clustering algorithm

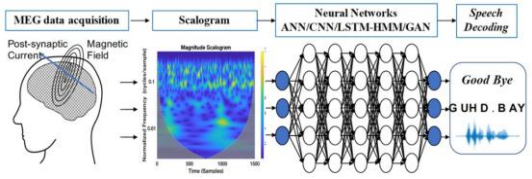


14x speedup
template matching routine

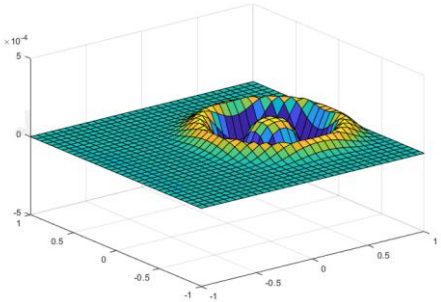
12x speedup
using Black-Scholes model



44x speedup
simulating the movement of celestial objects



10x speedup
deep learning training



77x speedup
wave equation solving

[Run MATLAB functions on a GPU]

NVIDIA Titan V GPU, Intel® Core™ i7-8700T Processor (12MB Cache, 2.40GHz)

NASA Langley Accelerates Acoustic Data Analysis with GPU Computing

Challenge

Accelerate the analysis of sound recordings from wind tunnel tests of aircraft components

Solution

- Use Parallel Computing Toolbox to process acoustic data
- Cut processing time by running computationally intensive operations on a GPU

Results

- GPU computations completed 40 times faster
- Algorithm GPU-enabled in 30 minutes
- Processing of test data accelerated

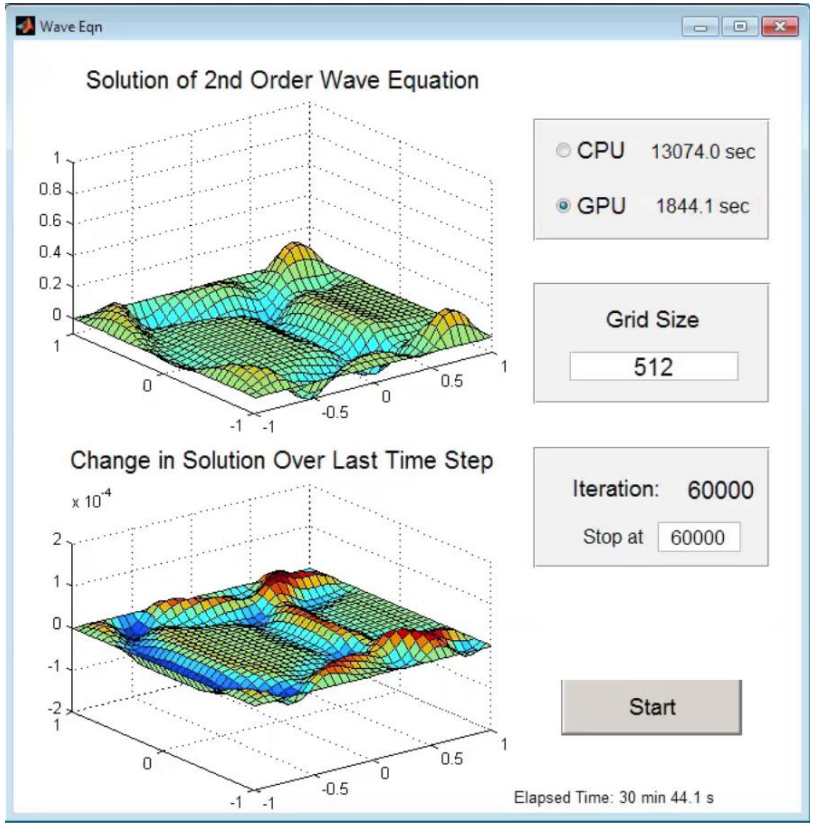
Wind tunnel test setup featuring the Hybrid Wing Body model (inverted), with 97-microphone phased array (top) and microphone tower (left).

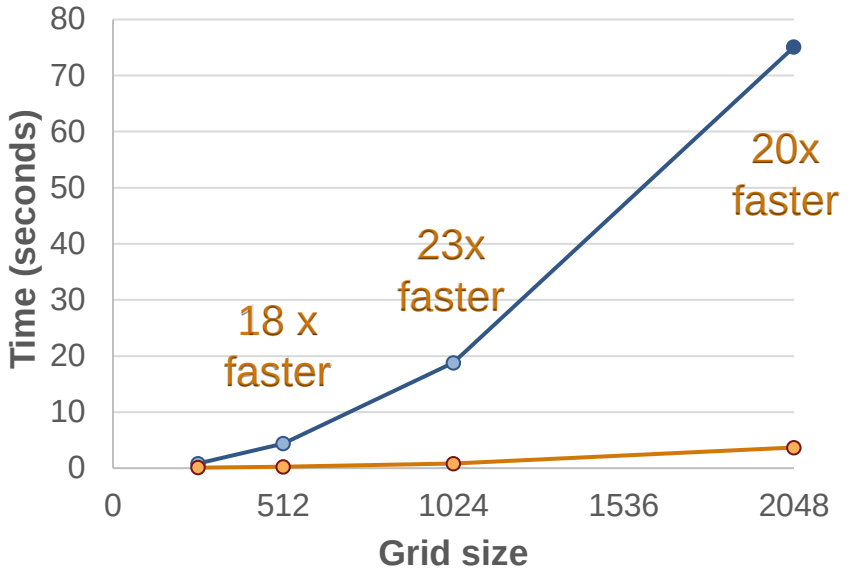
"Our legacy code took up to 40 minutes to analyze a single wind tunnel test. The addition of GPU computing with Parallel Computing Toolbox cut it to under a minute. It took 30 minutes to get our MATLAB algorithm working on the GPU—no low-level CUDA programming was needed."
- Christopher Bahr, research aerospace engineer at NASA

Link to user story

Run Same Code on CPU and GPU

Solving 2D Wave Equation

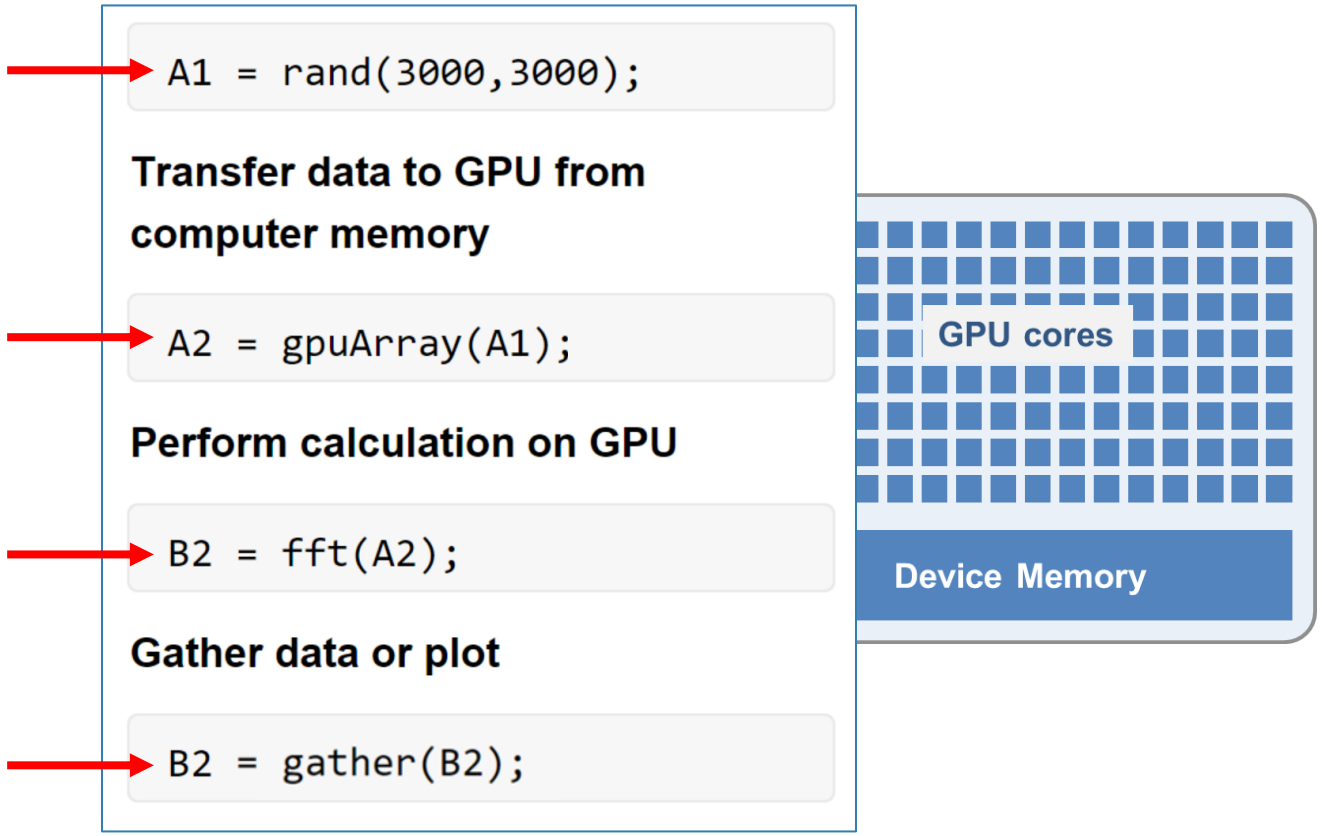




CPU	GPU
Intel(R) Xeon(R) W3550 3.06GHz 4 cores memory bandwidth 25.6 Gb/s	NVIDIA Tesla K20c 706MHz 2496 cores memory bandwith 208 Gb/s

Leverage your GPU to accelerate your MATLAB code

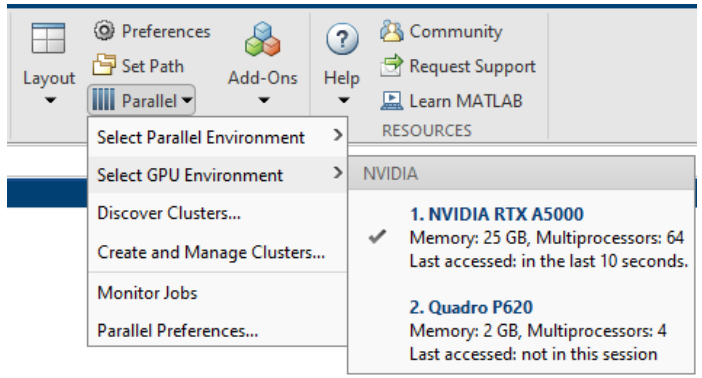
- Ideal Problems
  - Massively parallel and/or vectorized operations
  - Computationally intensive
- 800+ GPU-supported functions
- Use `gpuArray` and `gather` to transfer data between CPU and GPU



MATLAB GPU computing

Continued improvement to parallel control, usability, and performance

- Select GPU from Parallel menu



- gpuArray support – 15+ new features
- Performance enhancements for gpuArray

- Set preferred workers per profile
- Thread-based parallel support for 100+ additional features
- Distributed Array support – 4 new features, and new enhancements for conversion and distribution

Learn More

- MATLAB with GPUs

Outline

- Before we go parallel: Code optimization for better performance
- How to write and run parallel MATLAB code on your local machine or a cluster
- How to run MATLAB code on GPUs to accelerate your computations
- Use big data processing methods to handle large datasets
- Learning Resources

`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.)

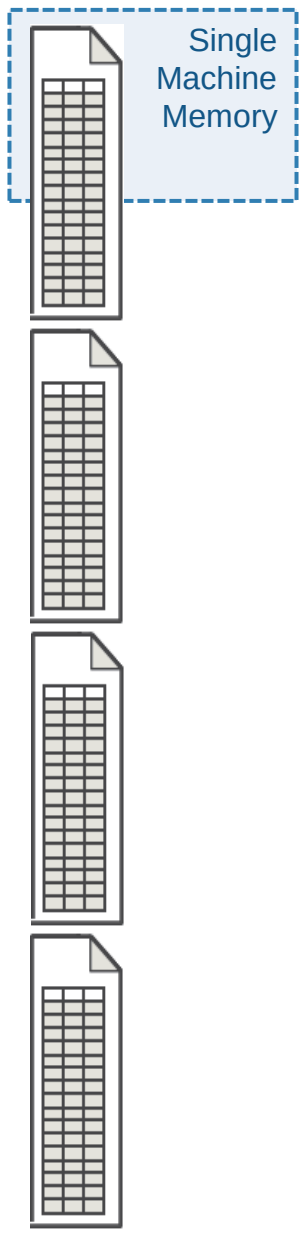
Working with tall arrays

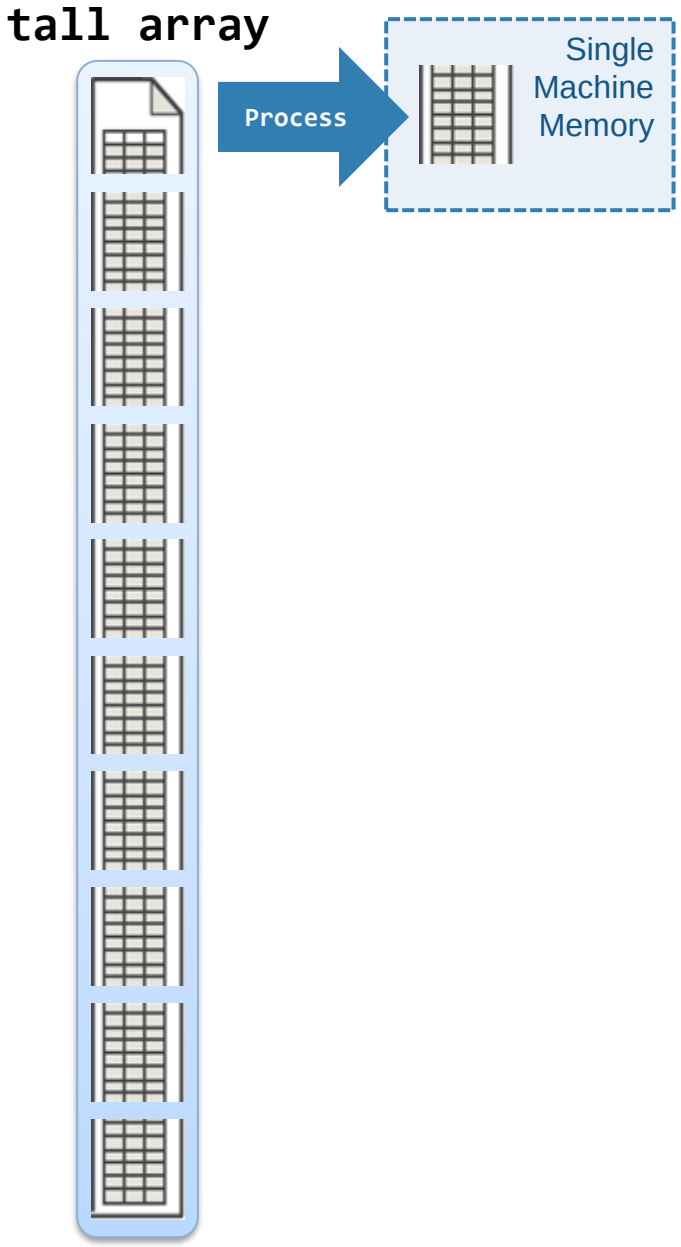
`tall` arrays

- Automatically breaks data up into small “chunks” that fit in memory
- Tall arrays scan through the dataset one “chunk” at a time

```
tt = tall(ds)
mDep = mean(tt.DepDelay,'omitnan')
mDep = gather(mDep)
```

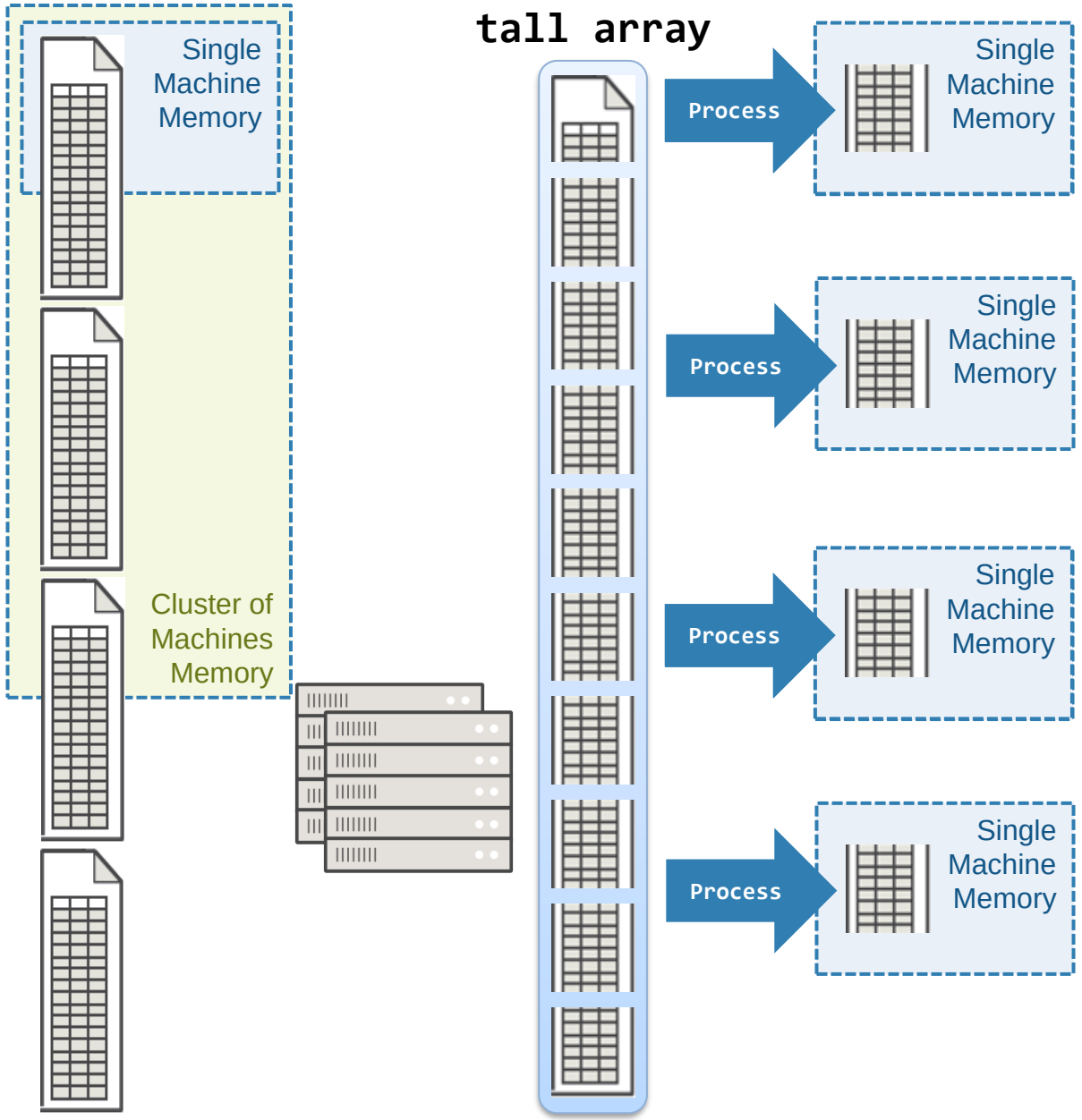
- Processing code for tall arrays is the same as ordinary arrays





`tall` arrays

- With Parallel Computing Toolbox, process several “chunks” at once
- Can scale up to clusters with MATLAB Parallel Server

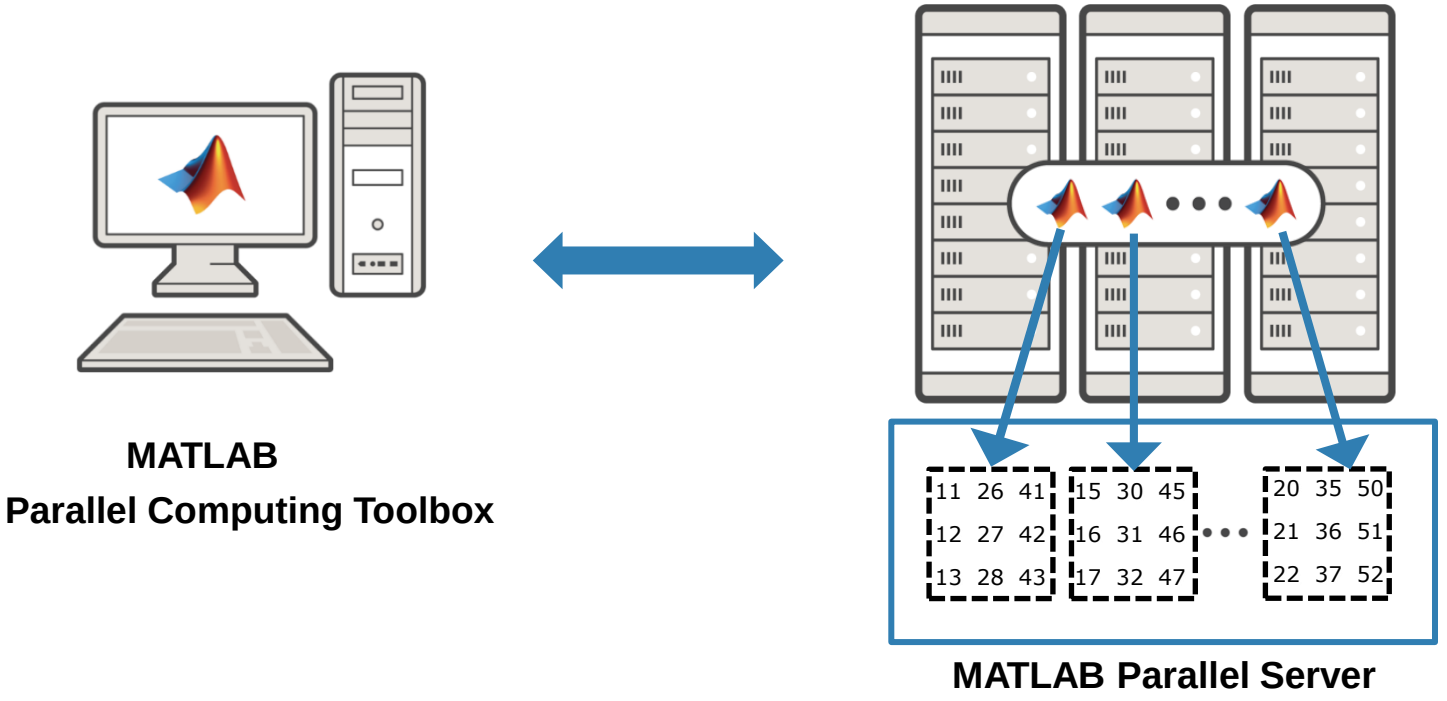


Demo: tall arrays

- https://www.mathworks.com/help/releases/R2023b/matlab/import_export/analyze-big-data-in-matlab-using-tall-arrays.html

`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



distributed arrays

Develop and prototype locally and then scale to the cluster

MATLAB
Parallel Computing Toolbox

```
% prototype with a small data set
parpool('local');

% Read the data - read in part of the data
ds = datastore('colchunk_A_1.csv');

% Send data to workers
dds = distributed(ds);

% Run calculations
A = sparse(dds.i, dds.j, dds.v);
x = A \ distributed.ones(n^2, 1);

% Transfer results to local workspace
xg = gather(x);
```

MATLAB Parallel Server

```
% prototype with a large data set
parpool('cluster');

% Read the data - read the whole dataset
ds = datastore('colchunk_A_*.csv');

% Send data to workers
dds = distributed(ds);

% Run calculations
A = sparse(dds.i, dds.j, dds.v);
x = A \ distributed.ones(n^2, 1);

% Transfer results to local workspace
xg = gather(x);
```

Working with distributed arrays

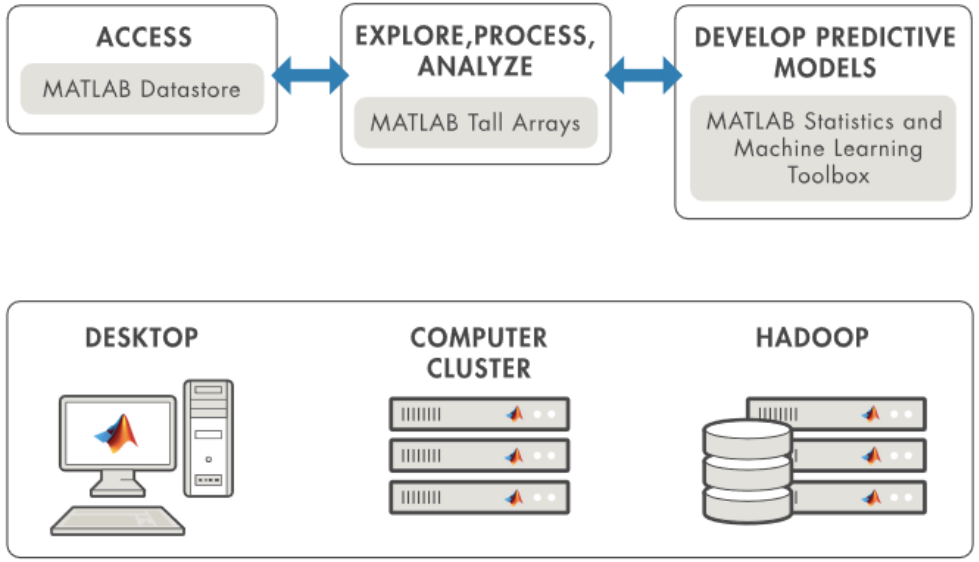
`tall` arrays vs. `distributed` arrays

- `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)
  - Create custom functions with `spmd` + `gop`

	Tall Array	Distributed Array
Support Focus	**Data Analytics, Statistics and Machine Learning**	**Linear Algebra, Matrix Manipulations**
Data Shape – Tall	✓	✓
Data Shape – Wide		✓
Prototype on Desktop	✓	✓
Helps on Desktop	✓	
Run on HPC	✓	✓
Run on Spark/Hadoop	✓	
Fault Tolerant	✓	

Learn More: Big Data

- Strategies for Efficient Use of Memory
- Resolving "Out of Memory" Errors
- Big Data with MATLAB
- MATLAB Tall Arrays in Action



Demo files

- https://mathworks-my.sharepoint.com/:f:/p/yueyixu/Er4mY1Ol8r5BooQT4eufh0AB-AEbn6G2dtqYqGI0M5CNZg?e=HWDbeC

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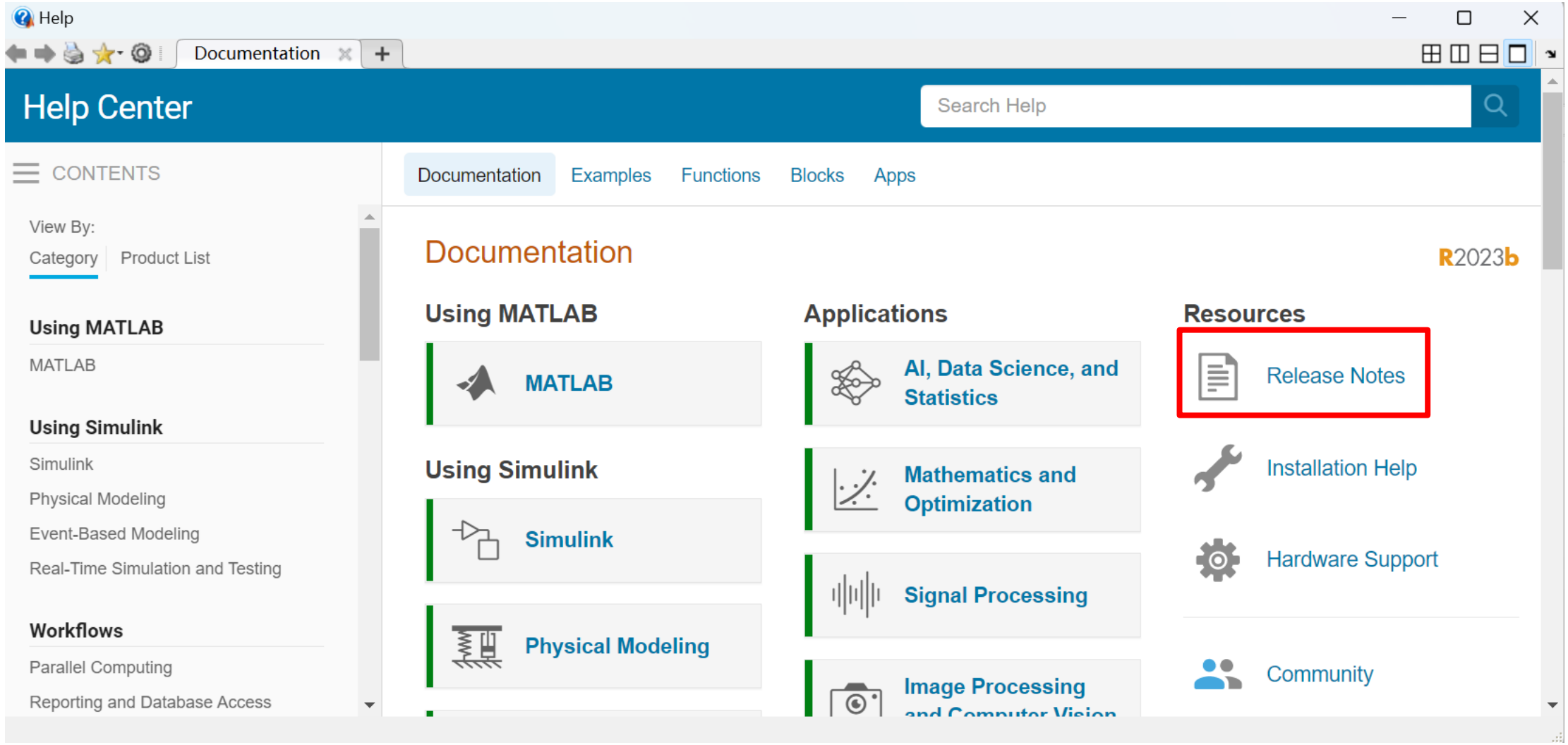
Documentation



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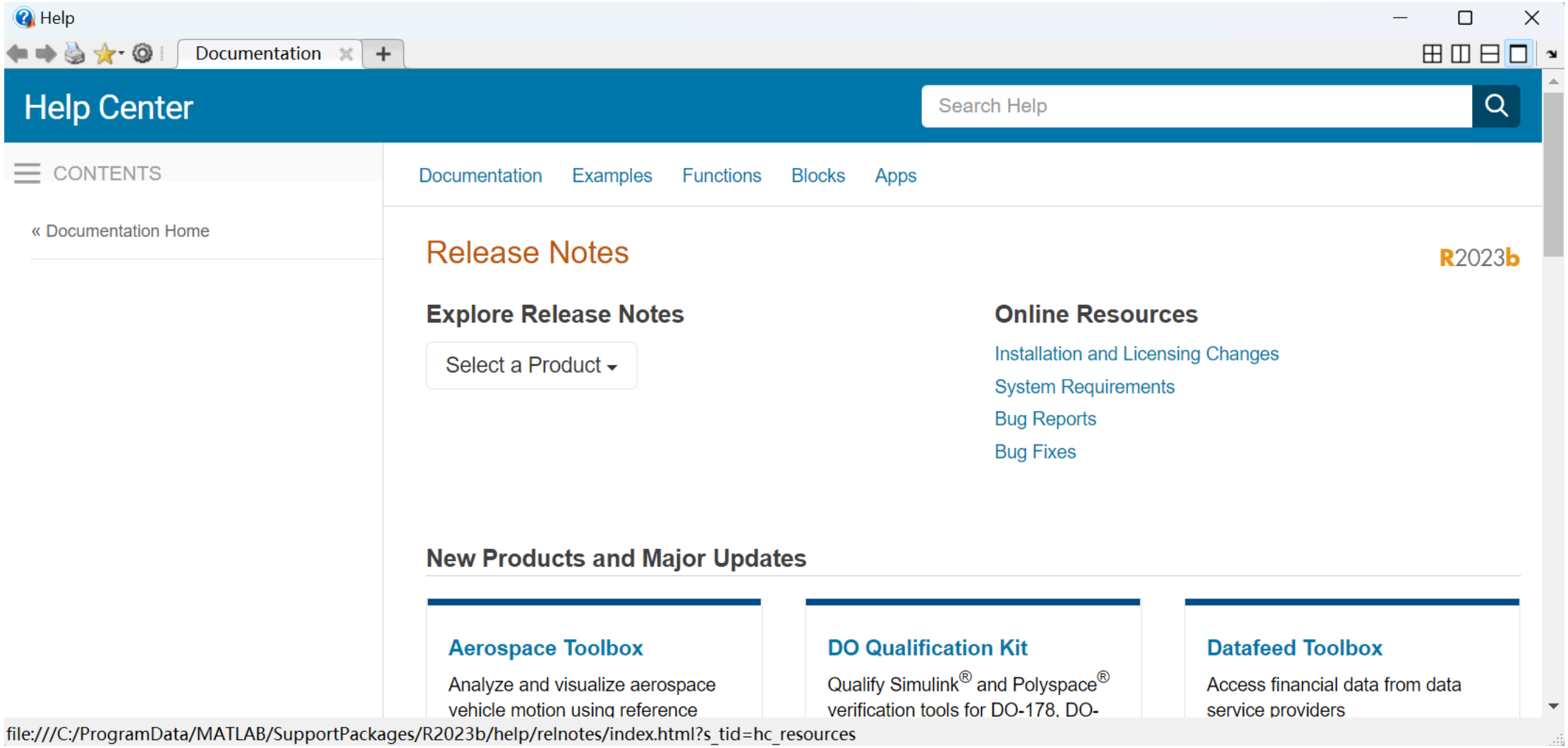
Release Notes



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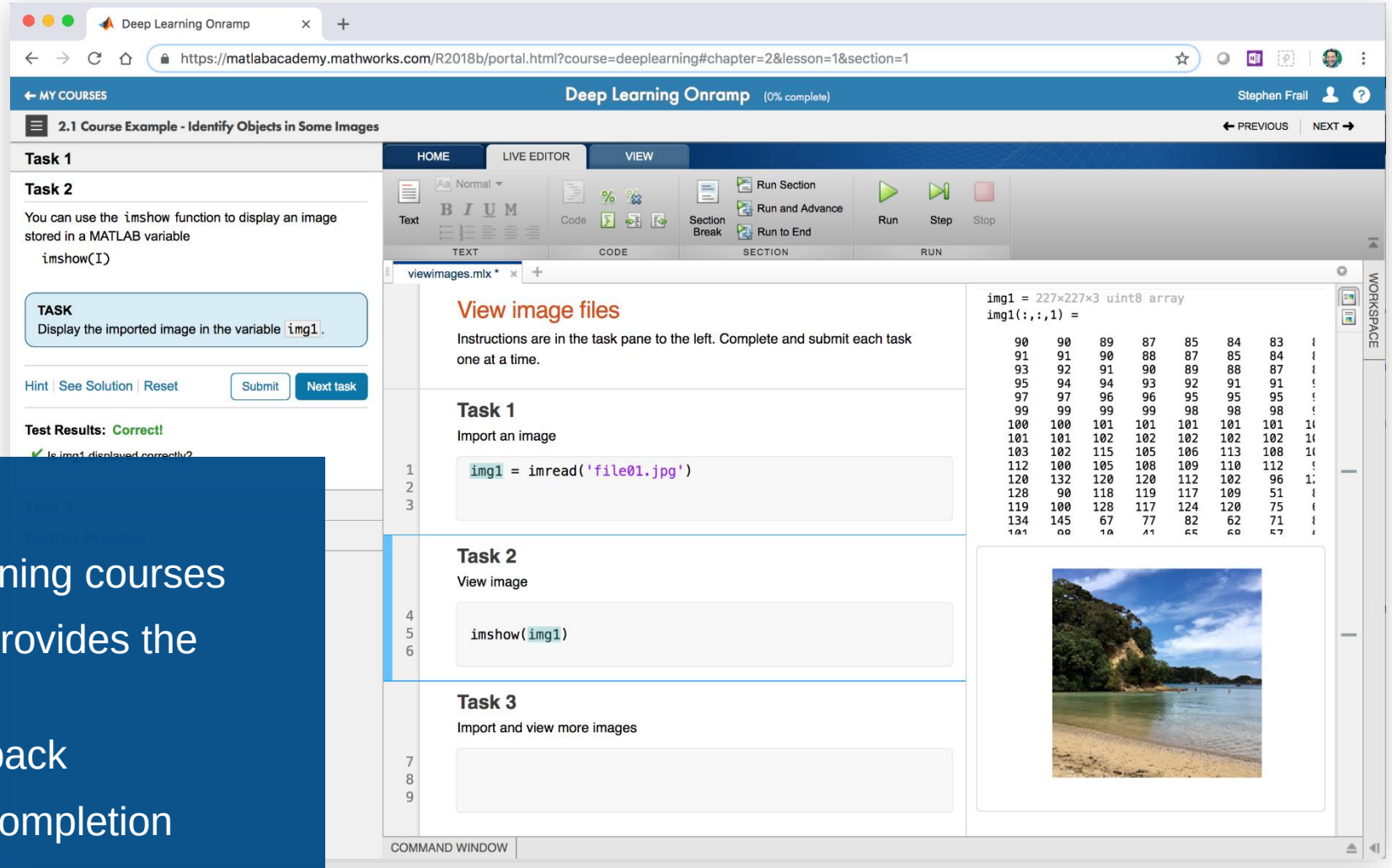

- High-quality, self-paced online training courses
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- 24/7 availability

Self-Paced Online Training Format and Learning Environment

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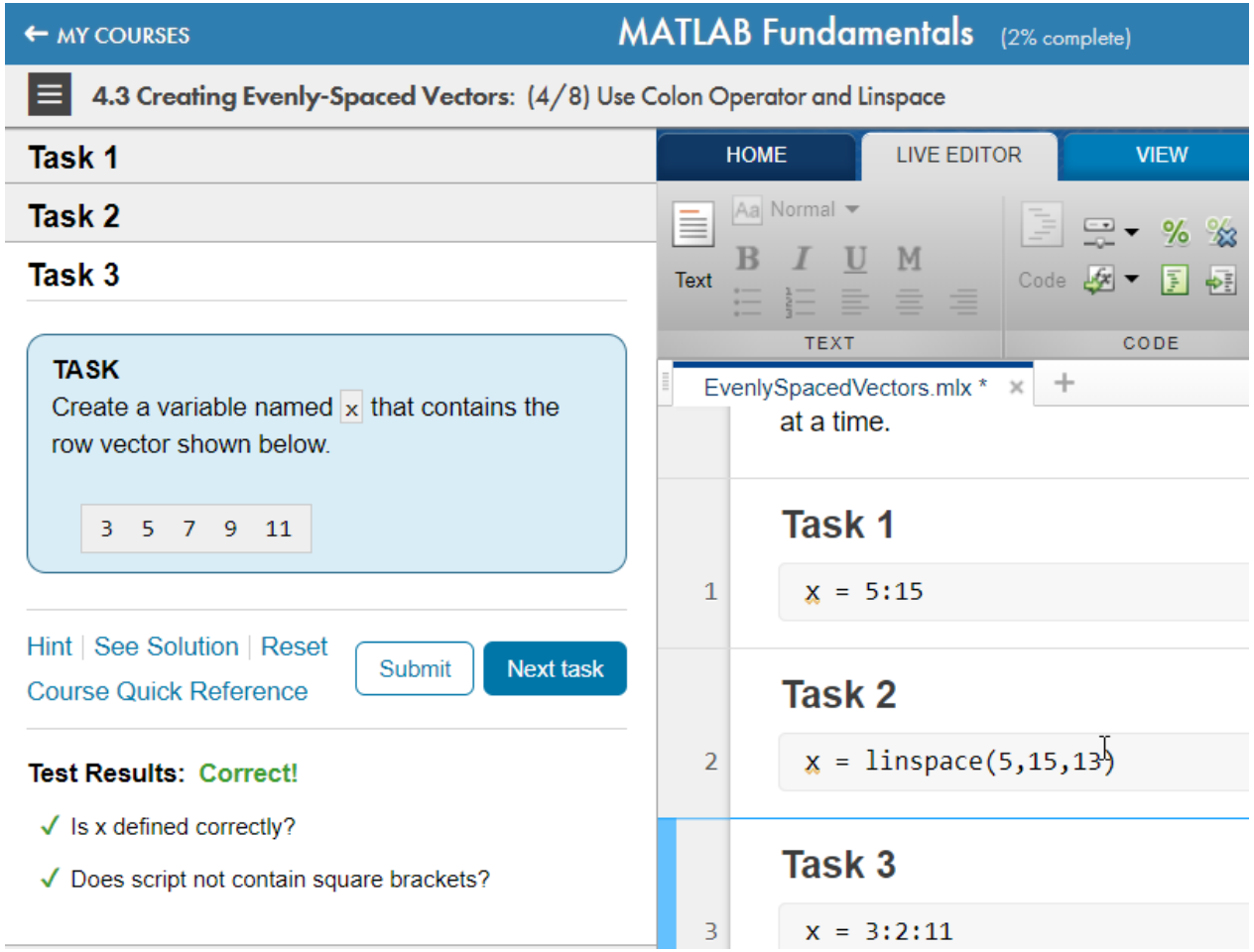
- Learn by doing: Complete tasks within MATLAB and Simulink. Receive immediate feedback
- Track progress and share certificate of completion



Self-Paced Online Courses

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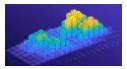
MATLAB and Simulink


MATLAB Fundamentals


Simulink Fundamentals


MATLAB Programming Techniques


MATLAB for Data Processing and Visualization

Image and Signal Processing


Image Processing with MATLAB

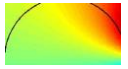

Signal Processing with MATLAB

Data Science and AI


Deep Learning with MATLAB


Machine Learning with MATLAB

Computational Mathematics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Q&A