

MATLAB: How to speed up your code and run jobs on Viking from MATLAB

Philip Harrison

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Today's talk



- Topic: Introduction on how to speed up your MATLAB code
- How to measure execution time
- Simple steps
 - Pre-assign arrays, vectorisation, built-in functions
- Use parallelisation
 - On your computer
- Use Viking
 - What is Viking?
 - Prerequisites and setup
 - Using Viking from within MATLAB
 - Getting data onto Viking
- Final comments

Why speed up your code?



- Who wants to wait for code to run?
- Faster code equals
 - More efficient use of time and resources
 - Get more research done
 - Use your computer for longer
 - Good habit to get into might not make much difference now, but could in the future
- Get the low hanging fruit first
- Strike a balance is the time you're spending to speed up your code longer than the time saved?

How to measure execution time



- How long does it take my code to run?
- Simple approach
 - Stopwatch tic and toc
- More complex approach
 - Code profiler
 - Simple to use 'Run and time'
 - Produces interactive report:
 - Execution time
 - Number of calls to a function
- Mathworks help: <u>Measure</u> performance of your program



Simple ways to speed up MATLAB code: Street of York Preallocate arrays

• Resizing arrays within a loop takes extra time to find more memory

tic x = 0;for k = 2:1000000 x(k) = x(k-1) + 5;end toc Elapsed time is 0.107429 seconds. tic x = zeros(1,100000);for k = 2:100000 x(k) = x(k-1) + 5;end toc Elapsed time is 0.017111 seconds.

- Version on right with preallocation approximately 6 times faster
- MATLAB will warn you in the code editor, code profiler and code analyser
- Mathworks help <u>Preallocating arrays</u>

Simple ways to speed up MATLAB code: Structure of York

- MATLAB optimised for vector and matrix operations
- Vector and matrix algebra and functions

```
tic
i = 0;
for t = 0:.01:10
    i = i + 1;
    y(i) = sin(t);
end
toc
VS
tic
t = 0:.01:10;
y = sin(t);
toc
Elapsed time is 0.006431 seconds.
```

Elapsed time is 0.013842 seconds.

- Version with vectorisation approximately 2 times faster
- Code is neater, more readable, fewer chances for bugs
- Mathworks help <u>Vectorization</u>

Simple ways to speed up MATLAB code: 😽 Use built-in functions

- Don't reinvent the wheel!
- Optimised for speed preallocation, vectorisation
- Written by MATLAB experts, refined over time
- Check available Toolboxes
 - All licensed ones should be installed on managed PCs
 - Add relevant toolboxes on unmanaged/personal devices
- Search Mathworks FileExchange
 - Community repository of code examples, functions, applications
 - <u>https://uk.mathworks.com/matlabcentral/fileexchange/</u>
- Search internet

Simple ways to speed up MATLAB code: Parallelisation

- Normal for loops executes the code sequentially
- parfor loops execute in parallel simultaneous execution!
- Can significantly speed up execution
- Can only use if each loop execution is independent of the others
- Useful for analysing multiple input data files or independent simulations
- Just swap for with parfor
- Uses the multiple cores in CPU of your computer
- Mathworks help <u>Decide when to use parfor</u>

Simple ways to speed up MATLAB code: Street of York Parallelisation

```
tic
tic
                                                               n = 200;
n = 200;
                                                               A = 500;
A = 500;
                                                               a = zeros(1,n);
a = zeros(1, n);
                                            VS
                                                               parfor i = 1:n
for i = 1:n
                                                                  a(i) = max(abs(eig(rand(A))));
   a(i) = max(abs(eig(rand(A))));
                                                               end
end
                                                               toc
toc
                                                               Elapsed time is 9.479539
Elapsed time is 21.236543 seconds
```

- Parallel version is 2 times faster with 4 cores
- Creates a parallel pool but this takes time to create for the first run (extra 60 seconds)

What is Viking?



- University of York's Research Computing Cluster
- Cluster = lots of computers working as a single system
- Free at the point of use
- Offload code execution from local computer to the cluster
- Typically use Linux command line to interact with it
- Submit 'jobs' requesting specific resources
 - Managed by Slurm workload manager and job scheduler
- Lots more information <u>Viking Wiki pages</u>

Viking & MATLAB Prerequisites



- Need to request access user to complete the <u>Viking User</u> <u>Application Form</u>
- But need a project code first supervisor/PI completes the <u>Viking</u> <u>Project Application Form</u>
- Can only connect to Viking from on-campus or via the VPN
- MATLAB Parallel Computing Toolbox on local MATLAB instance
 - Installed by default on managed devices and via Software Center
 - Personal devices make sure to add it
- Local MATLAB version that matches a version on Viking
 - Currently: 2018a, 2020a, 2020b, 2021a, 2022a

Cluster Profiles



- Need a Cluster Profile to tell MATLAB how to communicate with Viking
- Automatically generated using scripts <u>download scripts</u> from the <u>Viking MATLAB Wiki page</u>
 - Only tested on Windows so far, but should work for Linux and Mac
- Put scripts on local machine, make sure the location is in MATLAB's path, e.g.
 - o addpath(genpath('C:\Users\abc123\Documents\MATLAB\Viking'))
- Run creation script
 - configCluster
- Only information required is University username, e.g. abc123
- Creates a cluster profile called 'viking'

Cluster Profiles



📣 Cluster Profile Manager			– 🗆 X			
	🖉 🗈 Duralizate 🗛 Durana 🧀 🖌 🍪 Manage Lic	enses & Alerts				
Discover Add Cluster Create Cloud Import E Clusters Profile Cluster CREATE	idit Delete Set as Default Export MANAGE PROFILE VALIDATE CLOI	Connectivity er UD HELP				
Cluster Profile	viking		Type: Generic (<u>How to configure</u>)			
local (default)	Properties Validation					
viking			^			
	Description of this cluster Description	viking				
	Folder where job data is stored on the client JobStorageLocation	C:\Users\pth102\AppData\Roaming\MathWor	ks\MATLAB\generic_cluster			
	Number of workers available to cluster NumWorkers	512				
	Number of computational threads to use on each worker NumThreads	1 (default)				
	Root folder of MATLAB installation for workers ClusterMatlabRoot	/opt/apps/easybuild/software/MATLAB/2022a				
	License number (Optional: Used only if this cluster uses online licensing) LicenseNumber	<none> Fok Plu</none>	erontaining scheduler plugin scripts aginScriptsLocation	C:\Users\pth102\OneDrive -	University of York\Docume	ents\MATLAB\Viking\I.
		Add	ditional properties for plugin scripts	Name	Value	Туре
	Cluster uses online licensing	<none></none>	iteronartrobereres	AccountName		String ^
	RequiresOnlineLicensing			AdditionalSubmitArgs		String
				ClientConnectsToWorkers	true	Logical
	CLUSTER ENVIRONMENT			Constraint	Thangiyorkideluk	String
	Cluster nodes' operating system OperatingSystem	unix		EmailAddress		String v

Cluster Profile Validation



- Need to Check that the profile, your account and connection are working
- Parallel > Create and Manage Clusters
- Click 'Validation' tab not the 'Validate button'
- Update 'Number of workers to use' to 4
- Untick 'Parallel pool test (parpool)

Velideties		Type: Generic 1	(How to conligue
roperties validation			
Stage	Status	Description	
Cluster connection test (parcluster)	Not run		
Job test (createJob)	Not run		
SPMD job test (createCommunicatingJob)	Not run		
Pool job test (createCommunicatingJob)	Not run		
Parallel pool test (parpool)	Not run		





Cluster Profile Validation



M.C.L.	CI D
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- Click 'Validate' button
- Will be asked if using an identity file: No
- Will be asked for your university password
- Then wait! Successful validation looks like:

ser Cre	dentials		<u> </u>		×
Use	an identity file to login to viking.	york.ac.uk? S	elect "no" to u	se a	
pas	Yes	io Ca	ncel		
	👅 Enter password	-	×		
	Enter the password for us 'viking.york.ac.uk':	ser 'pth102'	on		



Demo time...



Useful commands



- c = parcluster('viking') creates a cluster object using the viking profile
- Modify and add properties with:
 - o c.AdditionalProperties.NumNodes = 1;
 - o c.AdditionalProperties.ProcsPerNode = 9;
- Submit jobs with batch
 - o myjob = batch(c, 'scriptname', 'pool', 8)
 - \circ Number of procs/workers requested must be 1 greater than specified with <code>pool</code>
 - Scripts are on local device and sent to Viking
 - Mathworks batch examples

Useful commands



- diary(myjob) returns elapsed time
- load (myjob) loads all workspace variables from specified job
- Job Monitor (Environment Toolbar > Parallel > Job Monitor)
 - Shows status of jobs
- Can submit job(s) then close MATLAB and jobs will run on Viking
- After reopening MATLAB get the results back using either:
 - Right-click on job ID in the Job Monitor window > Load Variables
 - Or

```
c = parcluster('viking');
job8 = findJob(c, 'ID', 8);
load(job8);
```

Getting data on and off Viking



• Windows: WinSCP

- In Software Center on managed PCs
- Personal devices download from https://winscp.net/eng/download.php
- Mac: Filezilla
 - Download from: https://filezilla-project.org/
- Use /scratch folder to store data
 - Fast
 - $\circ \quad \text{No limit on number of files} \\$
 - \circ 3 TB by default
 - WARNING scratch is not backed up

WinSCP			- 🗆 ×
Local Mark Files Commands Session Options R	iemote Help		
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Final comments



- Just an outline and introduction
- Lots of options and configurations
- Experiment find out what works/doesn't work
- Viking 2 is coming later in the year
 - Hopefully with automatic cluster discover!
- Using Linux commands are a useful complement to check on job progress, files etc

Sources of help & information



- Research Coding Club Slack channel and drop-in sessions
 - <u>Webpages with previous talks</u> e.g. Parallelisation
- Email to IT Support itsupport@york.ac.uk
- Mathworks help <u>Techniques for Improving Performance</u>
- MATLAB training:
 - MATLAB Onramp (2 hours)
 - MATLAB Fundamentals (16.5 hours)
 - MATLAB for Data Processing and Visualization (8 hours)
 - MATLAB Programming Techniques (16 hours)
 - Object-Oriented Programming Onramp (2 hours)



Questions?