

MATLAB on UL HPC Checkpointing & parallel execution

UL High Performance Computing (HPC) Team

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Latest versions available on Github:

UL HPC tutorials: UL HPC School:

https://github.com/ULHPC/tutorials

https://hpc.uni.lu/hpc-school

This tutorial's sources: https://github.com/ULHPC/tutorials/tree/devel/advanced/MATLAB2

















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1 Pre-requisites

2 Objectives

3 Checkpointing Example 1 revisited

Parallelization Example 2 revisited

5 Conclusion



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Sample MATLAB scripts used in the tutorial

download only the scripts:

(frontend)\$> mkdir \$HOME/matlab-tutorial2 (frontend)\$> cd \$HOME/matlab-tutorial2 (frontend)\$> wget https://raw.github.com/ULHPC/tutorials/devel/advanced/MATLAB2/code/example1.m (frontend)\$> wget https://raw.github.com/ULHPC/tutorials/devel/advanced/MATLAB2/code/example2.m (frontend)\$> wget https://raw.github.com/ULHPC/tutorials/devel/advanced/MATLAB2/code/google finance data.m

• or download the full repository and link to the MATLAB tutorial:

```
(frontend)$> git clone https://github.com/ULHPC/tutorials.git
(frontend)$> ln -s tutorials/advanced/MATLAB2/
$HOME/matlab-tutorial2
```





In order to see locally the MATLAB graphical interface, a package providing the X Window System is required:

- on OS X: XQuartz http://xquartz.macosforge.org/landing/
- on Windows: VcXsrv http://sourceforge.net/projects/vcxsrv/

Now you will be able to connect with X11 forwarding enabled:

- on Linux & OS X:
 - $\$ ssh access-gaia.uni.lu X
- on Windows, with Putty Connection \rightarrow SSH \rightarrow X11 \rightarrow Enable X11 forwarding



Pre-requisites



Checkpointing Example 1 revisited



5 Conclusion



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Better understand the usage of MATLAB on the UL HPC Platform

application-level checkpointing

 $\, \hookrightarrow \,$ using in-built MATLAB functions



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Better understand the usage of MATLAB on the UL HPC Platform

- application-level checkpointing
 - $\,\hookrightarrow\,$ using in-built MATLAB functions

• taking advantage of some parallelization capabilities

- $\, \hookrightarrow \, \text{ use of } \text{parfor} \,$
- \hookrightarrow use of GPU-enabled functions



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• taking advantage of some parallelization capabilities

- $\, \hookrightarrow \, \text{ use of } \text{parfor} \,$
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• adapting the parallel code with checkpoint/restart features

















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Technique for adding fault tolerance to your application. You adapt your code to (regularly) save a snapshot of the environment (workspace), and restart execution from the snapshot in case of failure.







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Technique for adding fault tolerance to your application. You adapt your code to (regularly) save a snapshot of the environment (workspace), and restart execution from the snapshot in case of failure.

Why make the effort to checkpoint?

- because your code may take longer to execute than the maximum walltime allowed
- because losing (precious) hours or days of computation when something fails may (should!) not be acceptable





• checkpointing (too) often can be counterproductive

- \hookrightarrow saving state in each loop may take longer than its actual computing time
- $\hookrightarrow\,$ saving state incrementally can lead to fast exhaustion of your \$HOME space
- \hookrightarrow in extreme cases can lead to platform instability especially if running parallel jobs!





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- \hookrightarrow in extreme cases can lead to platform instability especially if running parallel jobs!
- checkpointing (especially parallel) code can be tricky
- extra-care required if checkpointing simulations involving RNG (e.g. Monte Carlo-based experiments)
- ensure results consistency after you add checkpointing





1 Check that a checkpoint file exists:

exist('save.mat','file')

If it exists, restore workspace data from it:

load('save.mat')





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- 3 During computing steps, use control variables to direct (re)start of computation





- 1) Check that a checkpoint file exists: exist('save.mat', 'file')
- If it exists, restore workspace data from it: load('save.mat')
- 3 During computing steps, use control variables to direct (re)start of computation
- Every n loops, or if execution time (in loop or since startup) is above threshold, checkpoint:
 - $\hookrightarrow \text{ save full workspace state:} \qquad \qquad \texttt{save('save.tmp')}$
 - → save partial state: save('save.tmp', 'var1', 'var2')





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 - \hookrightarrow save full workspace state: save('save.tmp')
 - \hookrightarrow save partial state: save('save.tmp', 'var1', 'var2')
- Rename state file to final name:
 - system('mv save.tmp save.mat') \hookrightarrow this process ensures that in case of failure during checkpointing,
 - next execution doesn't try to restart from incomplete state



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- when (loop) execution time is above threshold (e.g. 1h):
 - \hookrightarrow use tic and toc stopwatch functions, remember they can be assigned to variables
 - $\,\hookrightarrow\,$ use the clock function
 - \hookrightarrow add some randomness to the threshold if you run several instances in parallel!



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 - \hookrightarrow use tic and toc stopwatch functions, remember they can be assigned to variables
 - $\,\hookrightarrow\,$ use the clock function
 - \hookrightarrow add some randomness to the threshold if you run several instances in parallel!
- every n loop executions
 - $\hookrightarrow\,$ remember that saving state takes time, depending on workspace size & shared filesystem usage, and
 - $\,\hookrightarrow\,$ if loops finish fast your code may be slowed down considerably
 - \hookrightarrow add some randomness to *n* if you run several instances in parallel!





Adding checkpointing to seq. code

example1.m: non-interactive script that shows:

• the use of a stopwatch timer

Checkpointing

- how to use an external function (financial data retrieval)
- how to use different plotting methods
- how to export the plots in different graphic formats

Tasks to tackle with checkpointing

- modify the script to download data for Fortune100 companies
- add & test checkpointing to save state after each company's data is downloaded
- more granular downloads modify download period from 1 year to 1 month, add & test checkpointing to save state after each download





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MATLAB on UL HPC



- Parallel Computing Toolbox http://www.mathworks.nl/help/distcomp/index.html
- Parallel for-Loops (parfor)

http://www.mathworks.nl/help/distcomp/getting-started-with-parfor.html

GPU Computing

http://www.mathworks.nl/discovery/matlab-gpu.html

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MATLAB on UL HPC



Option 1: Split input over several parallel, independent, MATLAB jobs \hookrightarrow great if it's possible (embarrassingly parallel problem)

Option 2: Use parfor to execute loop iterations in parallel

- \hookrightarrow single node only
- $\,\hookrightarrow\,$ we have 120 & 160 core nodes on which big problems can be tackled





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Option 3: Use GPU-enabled functions that work on the gpuArray data type

- \hookrightarrow require the code to be run on GPU nodes (subset of Gaia)
- \hookrightarrow great speedup for some workloads
- $\,\hookrightarrow\,$ 295 in-built MATLAB functions work on gpuArray

including discrete Fourier transform, matrix multiplication, left matrix division



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Option 4: MATLAB Distributed Computing Server (MDCS)

- $\, \hookrightarrow \, \text{ allows multi-node parallel execution} \,$
- $\,\hookrightarrow\,$ not yet part of the UL MATLAB license

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example2.m: non-interactive script that shows:

- the serial execution of time consuming operations
 - $\,\hookrightarrow\,$ the parallel execution and relative speedup vs serial execution
 - $\,\hookrightarrow\,$ setting the # of parallel threads through environment variables
 - $\, \hookrightarrow \, \, \mathsf{GPU}\text{-}\mathsf{based parallel execution}$







📅 🗖 Speed up your seq. code

example2.m: non-interactive script that shows:

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Tasks to tackle

- execute the script on regular vs GPU nodes (with different GPUs)
- increase # of iterations, matrix size
- increase # of workers with/without changing the # of requested cores
- modify the script with other GPU-enabled functions





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Parallelization Example 2 revisited





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MATLAB on UL HPC



- Checkpointing basics
- Specific MATLAB instructions for checkpointing
- Current MATLAB parallelization capabilities on UL HPC Platform

Perspectives

- (incrementally) modify your own MATLAB code for fault tolerance
- parallelize your own tasks using parfor/GPU-enabled instructions



Thank you for your attention...



Questions?

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Example 2 revisited





