MATLAB on UL HPC

Checkpointing & parallel execution



2015

SCHOOL





Valentin Plugaru

UL HPC Management Team, Parallel Computing and Optimization Group (PCOG), University of Luxembourg (UL), Luxembourg



Latest versions available on Github:

UL HPC tutorials:

 $\verb|https://github.com/ULHPC/tutorials||$

UL HPC School:

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

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





- Pre-requisites
- Objectives
- 3 Checkpointing Example 1 revisited
- Parallelization Example 2 revisited
- Conclusion





- Pre-requisites





Tutorial files

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/yahoo_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
```





X Window System

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







- Objectives







Objectives of this PS

Better understand the usage of MATLAB on the UL HPC Platform

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





Objectives of this PS

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 use of **parfor**
 - \hookrightarrow use of GPU-enabled functions





Objectives of this PS

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 use of **parfor**
 - \hookrightarrow use of GPU-enabled functions

adapting the parallel code with checkpoint/restart features







- 3 Checkpointing Example 1 revisited





School Checkpointing

What is it?

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.





Checkpointing

What is it?

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 pitfalls

- checkpointing (too) often can be counterproductive
 - → saving state in each loop may take longer than its actual computing time
 - → saving state incrementally can lead to fast exhaustion of your \$HOME space
 - running parallel jobs!





Checkpointing pitfalls

- checkpointing (too) often can be counterproductive
 - $\,\hookrightarrow\,$ saving state in each loop may take longer than its actual computing time
 - ⇒ saving state incrementally can lead to fast exhaustion of your \$HOME space
 - 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







Check that a checkpoint file exists:

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

load('save.mat')

If it exists, restore workspace data from it:

UNIVERSITÉ DU LUXEMBOURG





- Check that a checkpoint file exists: exist('save.mat', 'file')
- If it exists, restore workspace data from it: load('save.mat')
- During computing steps, use control variables to direct (re)start of computation







- Check that a checkpoint file exists: exist('save.mat', 'file')
- If it exists, restore workspace data from it: load('save.mat')
- 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:
 - → save full workspace state:

save('save.tmp')

→ save partial state:

save('save.tmp', 'var1', 'var2')





- Check that a checkpoint file exists:
 exist('save.mat', 'file')
- ② If it exists, restore workspace data from it: load('save.mat')
- Ouring computing steps, use control variables to direct (re)start of computation
- ② Every *n* loops, or if execution time (in loop or since startup) is above threshold, checkpoint:
 - → save full workspace state:

save('save.tmp')

→ save partial state:

save('save.tmp', 'var1', 'var2')

Rename state file to final name:

- system('mv save.tmp save.mat')
- this process ensures that in case of failure during checkpointing, next execution doesn't try to restart from incomplete state





When to trigger checkpointing?

- when (loop) execution time is above threshold (e.g. 1h):

 - \hookrightarrow use the clock function
 - → add some randomness to the threshold if you run several instances in parallel!





When to trigger checkpointing?

- when (loop) execution time is above threshold (e.g. 1h):

 - \hookrightarrow use the clock function
 - 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
 - → 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
- 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





- Parallelization Example 2 revisited





Reference documentation

- 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



Option 1: Split input over several parallel, independent, MATLAB jobs

→ great if it's possible (embarrassingly parallel problem)



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

 \rightarrow we have 120 & 160 core nodes on which big problems can be tackled





- Option 1: Split input over several parallel, independent, MATLAB jobs
 - → great if it's possible (embarrassingly parallel problem)
- Option 2: Use parfor to execute loop iterations in parallel
 - ⇒ single node only
 - \hookrightarrow we have 120 & 160 core nodes on which big problems can be tackled
- 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)
 - → 295 in-built MATLAB functions work on gpuArray

including discrete Fourier transform, matrix multiplication, left matrix division



- Option 1: Split input over several parallel, independent, MATLAB jobs
 - → great if it's possible (embarrassingly parallel problem)
- Option 2: Use parfor to execute loop iterations in parallel
 - ⇒ single node only
 - \hookrightarrow we have 120 & 160 core nodes on which big problems can be tackled
- 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)

 - → 295 in-built MATLAB functions work on gpuArray

including discrete Fourier transform, matrix multiplication, left matrix division

- Option 4: MATLAB Distributed Computing Server (MDCS)
 - → allows multi-node parallel execution
 - → not yet part of the UL MATLAB license

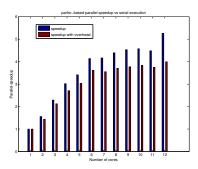




Speed up your seq. code

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
 - → GPU-based parallel execution







Speed up your seq. code

example2.m: non-interactive script that shows:

- the serial execution of time consuming operations
 - → the parallel execution and relative speedup vs serial execution
 - → setting the # of parallel threads through environment variables
 - → GPU-based parallel execution

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





- Conclusion





What we've seen in this session

- 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?

Valentin Plugaru

Mail: valentin.plugaru@uni.lu Office E-005 Campus Kirchberg 6, rue Coudenhove-Kalergi L-1359 Luxembourg

UL HPC Management Team mail: hpc-sysadmins@uni.lu













