UL HPC School 2017

PS8b: Advanced MATLAB (checkpointing and parallel jobs)

UL High Performance Computing (HPC) Team

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Latest versions available on Github:

UL HPC tutorials: https://github.com/ULHPC/tutorials

UL HPC School: http://hpc.uni.lu/hpc-school/

PS8b tutorial sources: https://github.com/ULHPC/tutorials/tree/devel/advanced/MATLAB1

Summary

1 **Pre-requisites**

2 Objectives

3 Checkpointing
Example 1 revisited

4 Parallelization
Example 2 revisited

5 Conclusion

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/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
```

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 → SSH → X11 → **Enable X11 forwarding**

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Objectives of this PS

Better understand the usage of MATLAB on the UL HPC Platform

- application-level checkpointing
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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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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
  - ↪ in extreme cases can lead to platform instability – especially if running parallel jobs!

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- 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

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4. 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')`

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5. 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):
  - ↪ use `tic` and `toc` stopwatch functions, remember they can be assigned to variables
  - ↪ use the `clock` function
  - ↪ add some **randomness** to the threshold if you run several instances in parallel!

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  - ↪ use the `clock` function
  - ↪ add some **randomness** to the threshold if you run several instances in parallel!
- every *n* loop executions
  - ↪ 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
  - ↪ 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

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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

Accelerate the time to result

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

$\hookrightarrow$ great **if** it's possible (embarrassingly parallel problem)

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↪ single node **only**

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

- ↪ **require** the code to be run on GPU nodes (subset of Gaia)
- ↪ **great speedup** for some workloads
- ↪ **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)

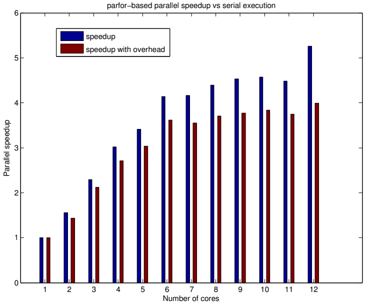
↪ allows multi-node parallel execution

↪ **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
  - ↪ the parallel execution and relative speedup vs serial execution
  - ↪ setting the # of parallel threads through environment variables
  - ↪ GPU-based parallel execution



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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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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?

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