Uni.lu HPC School 2019

PS07: Scientific computing using MATLAB

Uni.lu High Performance Computing (HPC) Team

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http://hpc.uni.lu

Latest versions available on Github:

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

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

PS07 tutorial sources:

https://ulhpc-tutorials.rtfd.io.rtfd.io/en/latest/maths/matlab/basics/

Summary

Session Objectives

Better understand the usage of MATLAB on the Uni.lu HPC Platform

- running in interactive mode
  - ↪ with either the full graphical or the text-mode interface
  - ↪ graphical web portal based on OnDemand coming soon

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  - ↪ example launchers for SLURM

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- using script (.m) files
- plotting data, saving the plots to file

Summary

Tutorial files

Sample MATLAB scripts used in the tutorial

- download only the scripts

```
mkdir $HOME/matlab-tutorial
cd $HOME/matlab-tutorial
wget https://raw.github.com/ULHPC/tutorials/devel/maths/\
     matlab/basics/code/
                          example1.m
                          example2.m
                          google_finance_data.m
                          file_data_source.m
                          AAPL.csv
```

- *or* download the full repository and link to the MATLAB tutorial

```
git clone https://github.com/ULHPC/tutorials.git
ln -s tutorials/maths/matlab/basics $HOME/matlab-tutorial
```

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:
  - ↪ in combination with Putty: **VcXsrv** http://sourceforge.net/projects/vcxsrv/
  - ↪ with MobaXTerm: nothing additional needed

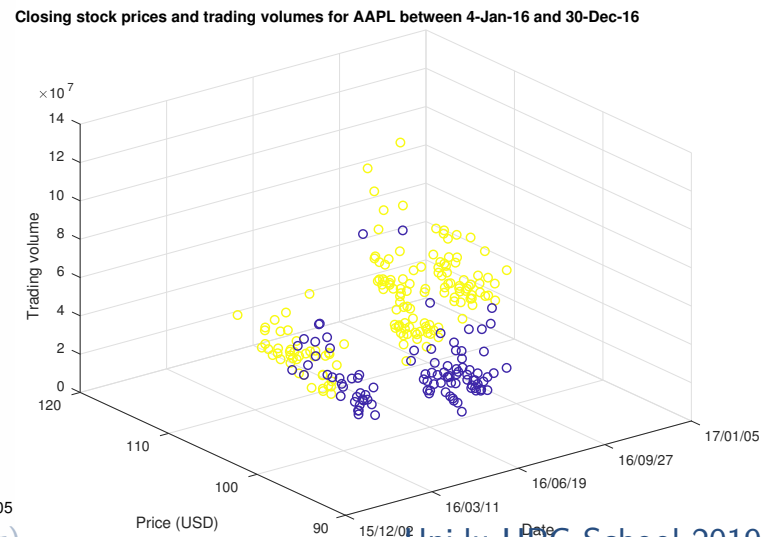
Now you will be able to connect with X11 forwarding enabled:

- on Linux & macOS: `ssh iris-cluster -X`
- on Windows
  - ↪ with Putty: Connection → SSH → X11 → **Enable X11 forwarding**
  - ↪ with MobaXTerm: remote GUI applications should work by default

Scripts and plots

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



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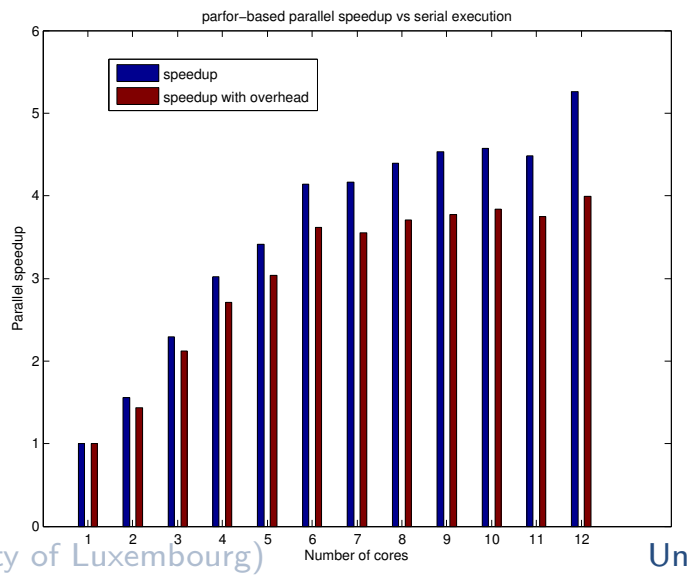

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- adapting parallel code with checkpoint/restart features

Checkpointing

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Technique for adding fault tolerance to your application.

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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 PRNG (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')`
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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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- 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

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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

Ref. documentation - parallelization

- **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
- Multi-GPU computing examples

  https://nl.mathworks.com/help/parallel-computing/examples/

  run-matlab-functions-on-multiple-gpus.html

Accelerating the time to result

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

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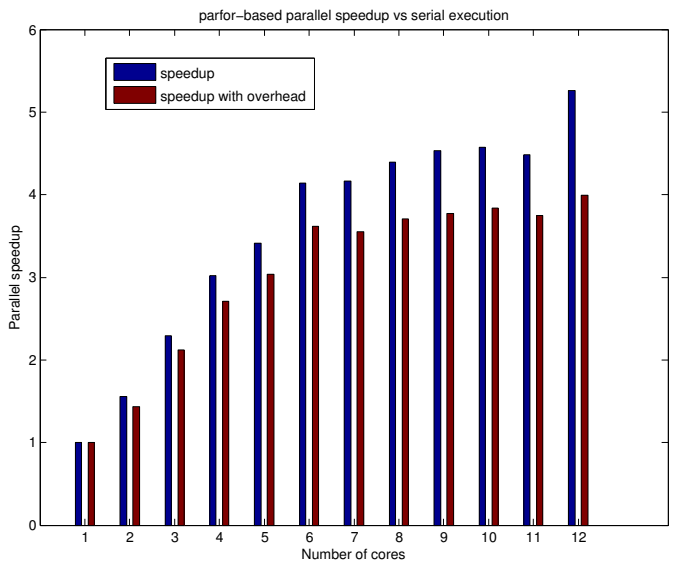

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Tasks to tackle

- execute the script on regular vs GPU nodes (with diff. GPUs)
- increase # of iterations, matrix size
- increase # of workers with/out changing # of req. cores
- modify the script with other GPU-enabled functions

Summary

Exercises - your mission today

- Read and understand the MATLAB tutorial

  https://github.com/ULHPC/tutorials/tree/devel/maths/matlab

  ↪ all provided scripts are fully commented
- Run all the examples
  - ↪ launching interactive/passive mode MATLAB
  - ↪ plotting script
  - ↪ parallel execution script

Useful links

- Getting Started with Parallel Computing Toolbox

  http://nl.mathworks.com/help/distcomp/getting-started-with-parallel-computing-toolbox.html

- Parallel for-Loops (parfor) documentation

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- Multi-GPU computing examples

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What we've seen so far (I)

- MATLAB execution modes on the Uni.lu HPC Platform
- Checking for available toolboxes and licenses
- Basics of plotting

Perspectives

- Personalize the UL HPC launchers with the MATLAB commands
- Check example #2 M-file for insight into basic parallel execution
- Parallelize your own tasks using parfor/GPU-enabled instructions

What we've seen so far (II)

- Checkpointing basics
- Specific MATLAB instructions for checkpointing
- MATLAB parallelization capabilities

Perspectives

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

Questions?

http://hpc.uni.lu

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