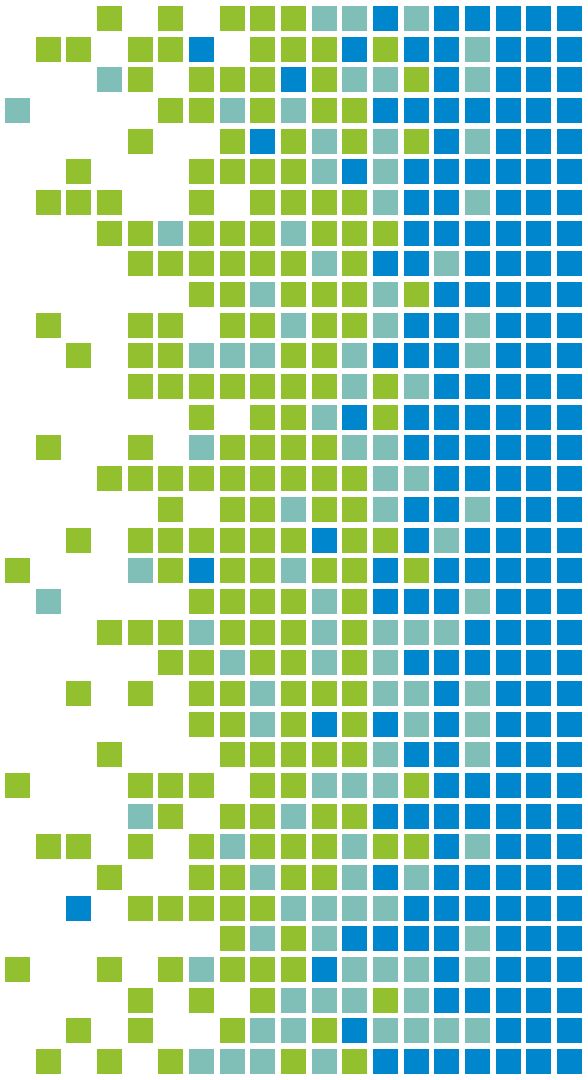
Introduction to HPC

Conda Environments



Agenda

Time	Topics
14:00 – 14:30	Introduction
14:30 – 15:00	Live demo
15:00 – 15:30	BREAK
15:30 – 16:00	Practical

Movitation

- We have developed a DL model
- Have a jupyter notebook with python code
- Takes too long to run locally
- Want to move it to Kay and run on the GPU nodes

4 Steps

- Copy notebook across to Kay
- Create conda environment
- Convert notebook form to plain python
- Create a SLURM script to run python code

Step One - Copy

- Copy notebook across to Kay
- Use scp or other

Step 2 – Conda

- Kay has base python environment
- Functionality is limited
- Conda allows multiple python versions and environments to co-exist
- Only one environment is active

Conda Environment

- Create an empty environment
- Add packages
- To use it it must be the active environment

Step 3 – Plain Python

- A jupyter notebook is a mix of text and code cells
- Very useful for teaching but is inherently interactive
- It is possible to run the notebook form on Kay
- Not suitable for long jobs
- Plain python can be run non-interactively

Step 4 – SLURM

- Kay is a multi-user machine
- Non-interactive jobs are scheduled to run
- Bash scripts allow non-interactive execution of applications
- SLURM is the scheduler and SLURM scripts have additional information for the scheduler

Live Demo

- Never ever do live demos!
- In classic Catch-22 style
- Here’s a live demo

Links

- This course
- https://www.ichec.ie/academic/national-hpc/documentation/tutorials/notebook-to-plain
- Using jupyter notesbooks on Kay
- https://www.ichec.ie/academic/national-hpc/documentation/tutorials/using-jupyter-notebook-kay-jupyter-hub

Live Demo (Notes)

- Need cuda+gcc modules
- Pip install tensorflow_gpu==2.3.1
- Pip install ipython and nbconvert