AIST4010 Spring2023 Tutorial 2

-- Frequently used tools

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Outline

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  - Usage example
- Pytorch
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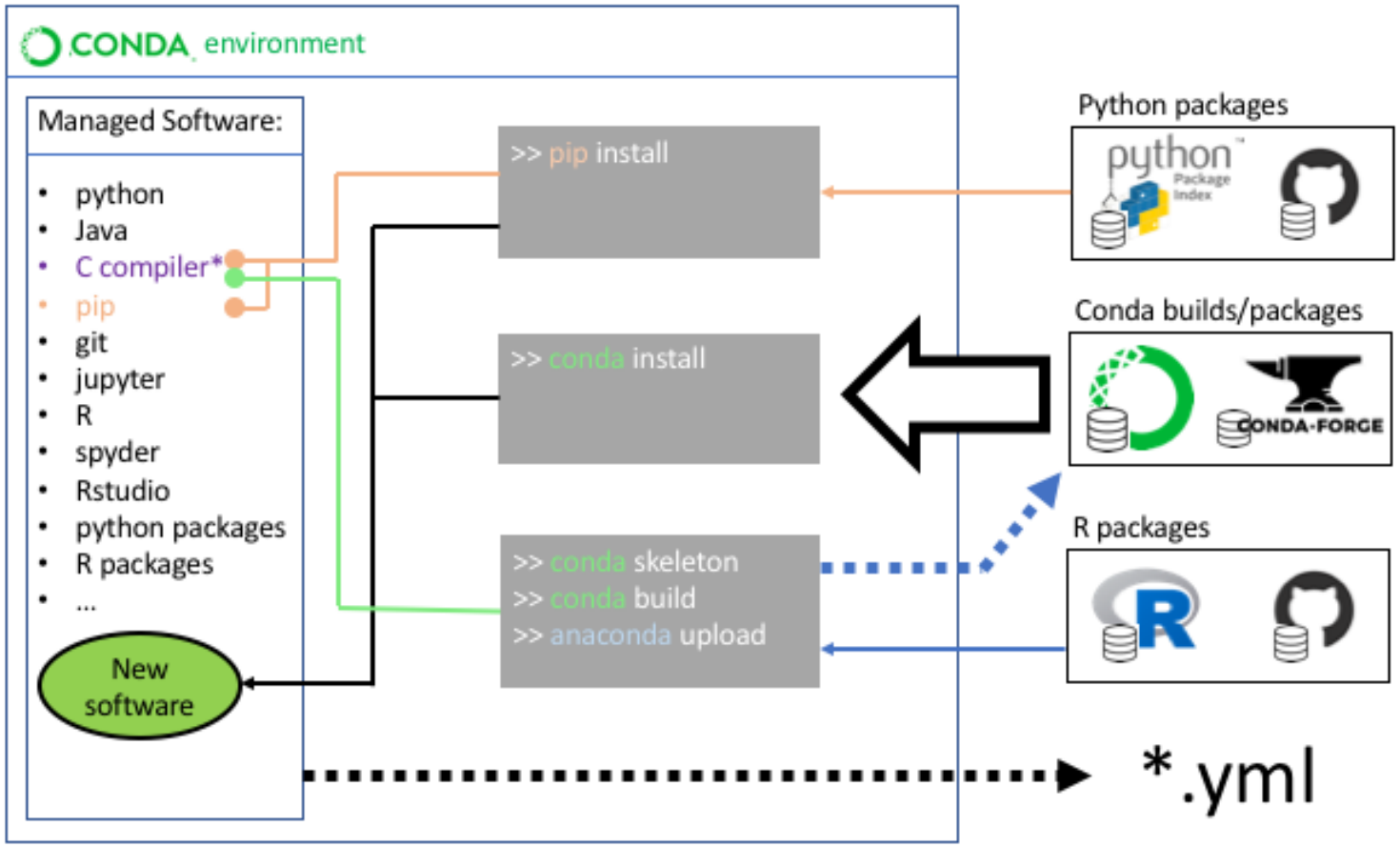
Conda VS Pip

	conda	pip
install python package	✅	✅
create virtual environment	✅, built-in	❌, requires `virtualenv` or `venv`
package format	`.tar.bz2`, `.conda`	`.whl`, `.tar.gz`
manages	binaries	wheel or source
can require compilers	❌	✅
package types	any	Python-only
dependency checks	✅	❌
package sources	Anaconda repo and Anaconda cloud	PyPI

https://www.anaconda.com/blog/understanding-conda-and-pip

Conda VS Pip



https://www.datisticsblog.com/2018/08/conda1/

Conda basic usage

Install and Manage Packages in Python

pip	conda
pip search pyserial	conda search pyserial
pip install pyserial	conda install pyserial
pip install pyserial --upgrade	conda update python
pip list	conda list

https://gallerylokasin.weebly.com/conda-install-package-inequality-version.html

Conda frequent commands

conda create --name $NAME

conda install --file $FILE

conda install $PACKAGE -c $SOURCE

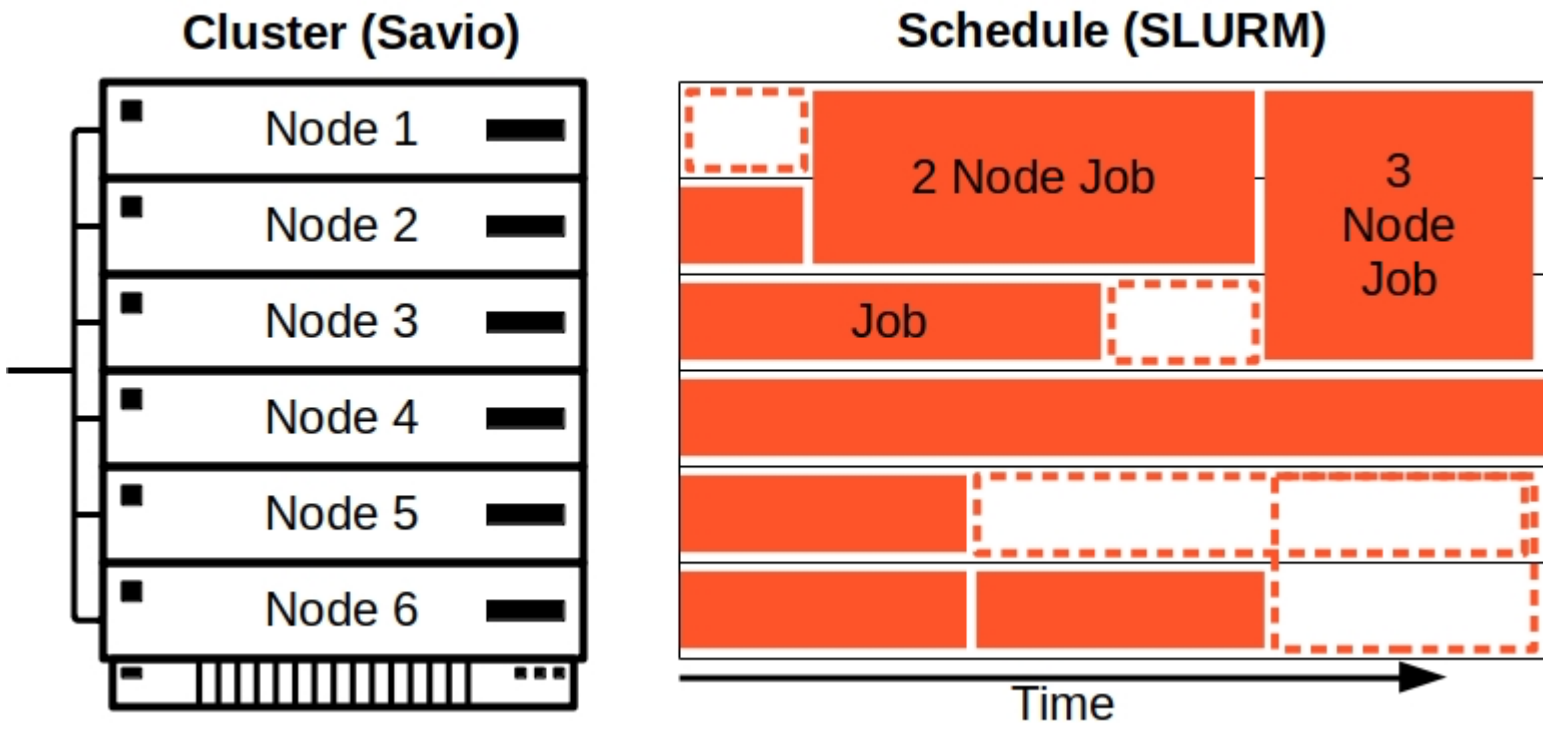
conda activate $NAME

conda update --all

conda list --export $FILE

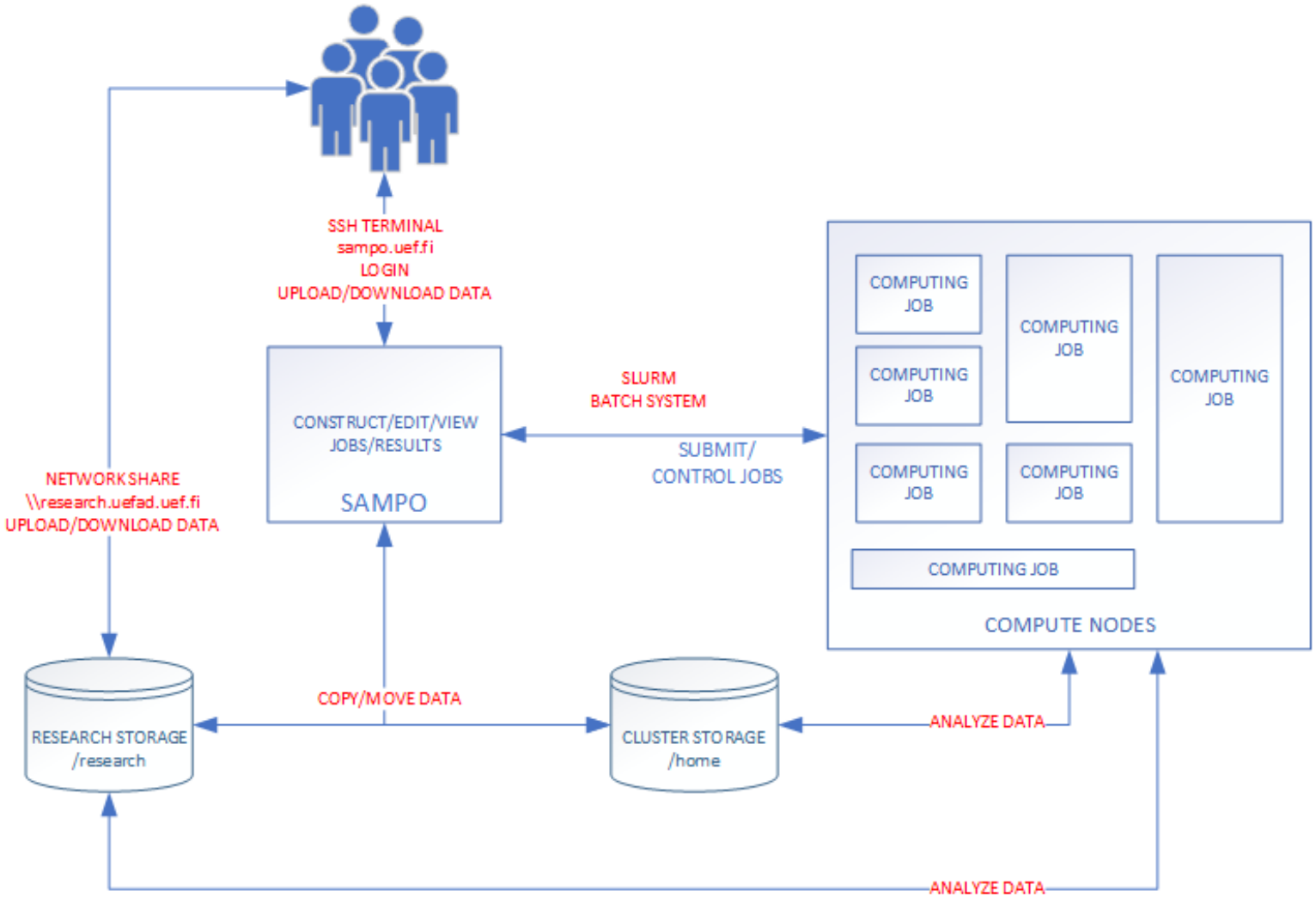
conda clean -pt

Slurm overview



https://docs-research-it.berkeley.edu/services/high-performance-computing/user-guide/running-your-jobs/why-job-not-run/

Slurm overview



Slurm usage

- Job submission
  - srun: submit a single job to run
  - sbatch: submit a batch of jobs (recommended, using submission script)
- Interactive (log into the node)
  - -> same as using a server
- Check resource
  - squeue: check the queue
  - sinfo: check available resource

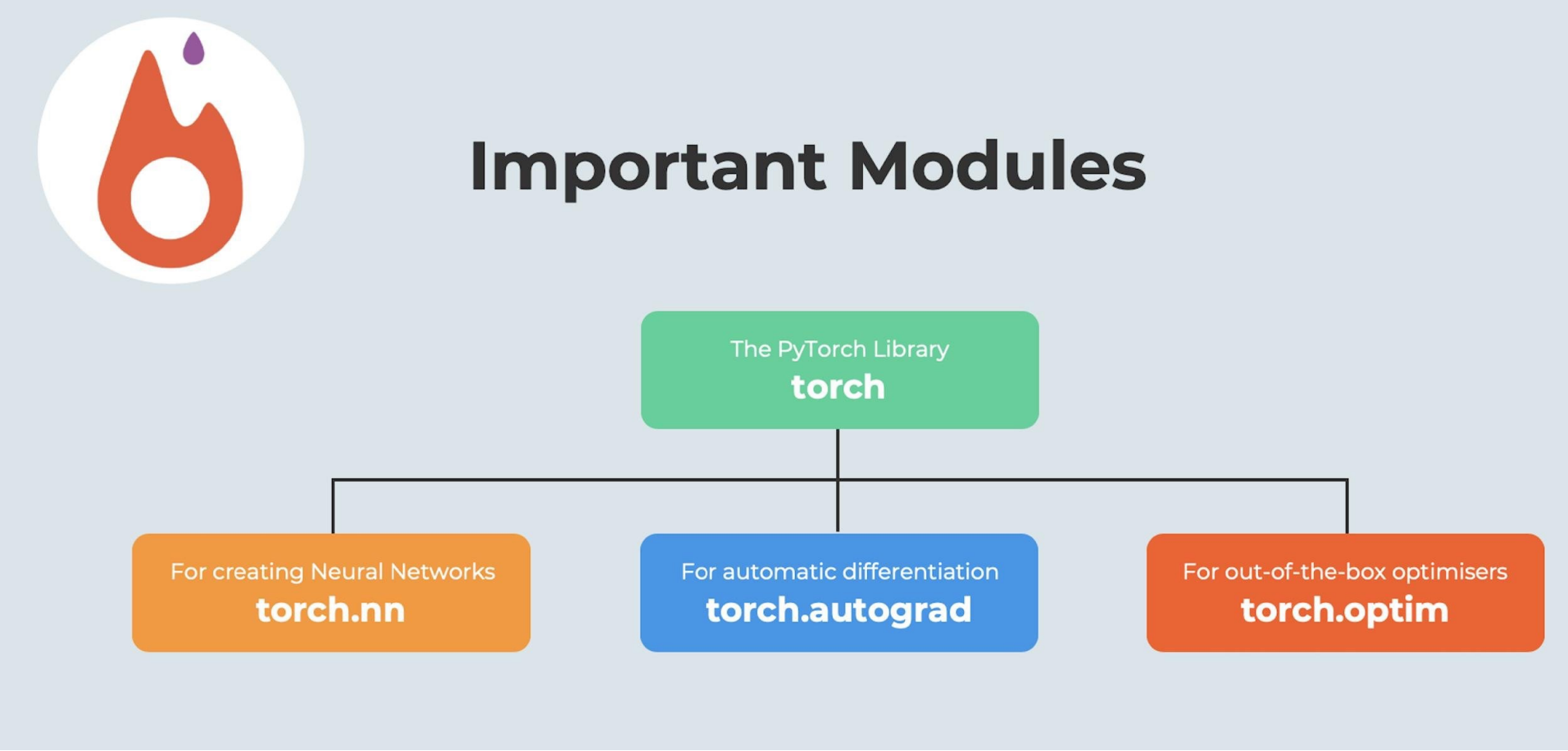
Slurm script example

SHELL |

```
#!/bin/bash

#SBATCH --job-name=maxFib       ## Name of the job
#SBATCH --output=maxFib.out     ## Output file
#SBATCH --time=10:00            ## Job Duration
#SBATCH --ntasks=1              ## Number of tasks (analyses) to run
#SBATCH --cpus-per-task=1       ## The number of threads the code will use
#SBATCH --mem-per-cpu=100M      ## Real memory(MB) per CPU required by the job.

## Load the python interpreter
module load python

## Execute the python script and pass the argument/input '90'
srun python script.py 90
```

REMINDER! If you have conda environment set up, please skip line `module load` and specify the python path of your env

Pytorch overview



Pytorch usage

- Create tensor or tensor manipulation
  - torch.matmul etc.
  - torch.tensor
- Build model
  - Model definition: torch.nn.Linear etc.
  - Loss definition: any operation or torch.nn.MSELoss etc.
- Train model
  - Optimizer definition: torch.nn.optim.Adam
  - Train/evaluation loop
  - Loss.backward() optimizer.step() optimizer.zero_grad()