The Scientific Computing Core
And how to use resources at FI?

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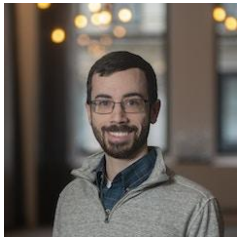
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Our mission

Core IT

ITSupport@simonsfoundation.org

Corporate computing

- General IT problems
- Printers
- Office/productivity software licenses
- Email problems
- WiFi
- Mac support

Scientific Computing Core (SCC)

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#scicomp

Scientific and technical computing

- Questions about the Linux clusters
- Package and configuration management on cluster
- Technical software and performance
- I/O and data storage
- Interactive data visualization and exploration workflows
- UI/UX
- Workstations support

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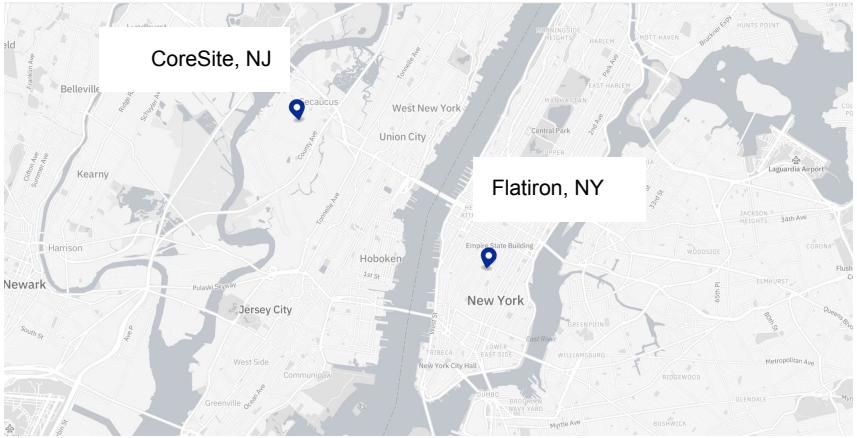
Where are our clusters?



Rusty

A cluster on two sites !?

- New York (Flatiron Institute)
- Seacaucus, NJ (CoreSite)
- Connected by dark fiber (1.6TB/s)

Popeye

- San Diego Supercomputing Center (La Jolla, CA)

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Clusters technical details

Rusty @ Flatiron

- 2 login nodes
- 440 CPU nodes
- 24 GPU nodes
- 4 Large memory nodes

Rusty @ CoreSite

- 2 login nodes
- 856 CPU nodes
- 123 GPU nodes

Popeye @ SDSC

- 2 login nodes
- 900 CPU nodes
- 32 GPU nodes
- 1 Large memory node

Total:
157k+ CPU cores
5M+ GPU cores

Cluster technical details (2): shared storage

Your **home** folder: (**/mnt/home/LOGIN**)

- Quota 1TB, 1M files
- Backed-up daily
- **Documentation and code**

Ceph: ~4000 drives (**/mnt/ceph/users/LOGIN**)

- No limit per user, but be a good citizen:
  - Contact us if you need to write 10+ TB
- **Simulation files, data**

Side note: local storage exists for tmp files!

On nodes: /tmp

What you will be using this summer

- CPU nodes:
  - Popeye has all Intel CPUs: from skylake to icelake, InfiniBand-connected
  - Rusty has both AMD (rome) and Intel (skylake and icelake). Mostly InfiniBand connected, but skylake's are on OmniPath
    - Check the wiki for details!
- If the code is heavily optimized, think about using AVX512 on the Intel nodes (check with the devs!)
- For multi-node jobs, make sure to put a constraint on the fabric. Eg: `-C rome,ib`

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Loading the software you need

- For most of the scientific packages presented during these BPM series, you will use the instructor-provided commands

- However for other software, you will be using modules
- Important things to remember:
  - **`module load module_name`** to load a module
  - **`module spider module_name`** to look for a module
  - **`module list`** to see what is currently loaded

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Modules examples: paraview, blender

As many of you will be using these packages during the summer, these are available in modules already:

```
$ module load python/3.9
$ module load paraview
```

The current version of modules does not support blender, but you can use the previous one:

```
$ module load modules/2.0
$ module load blender
```

Python

- If you need Python, always use the one from modules!

```
module load python
```

- If you need more packages than what is preinstalled, use virtual environments:

```
python -m venv ~/venvs/my_venv --system-site-packages
```

- conda should be use only as a last resort (otherwise the 1 million files limit might kick in for your home directory)

Resource Scheduling

In order to spread the compute resources:

- We use a batch scheduler: Slurm
- Check the documentation for samples
- You can also use it to reserve interactive sessions

- **Avoid launching hundreds of jobs simultaneously**
- **If you need many independent small jobs, try disBatch**
- **Do not use auto-submit scripts. Contact us for alternatives**

Some tips…

- For parallel codes, it is always a good idea to leave a couple of cores to the Operating System
  - On icelake, use 60 out of 64 cores
  - On rome, use 120 out of 128 cores
- Before you launch a week-long run, try to benchmark under different running conditions to find the best one!
  - Processor type?
  - Number of nodes/Number of cores?
  - Libraries?

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Take-home information

- The fundamentals: **Ceph - Modules - Slurm**

- Documentation: https://wiki.flatironinstitute.org
- scicomp@flatironinstitute.org
- #scicomp Slack channel

- Sciware sessions (Next one: Wednesday afternoon: GitHub)
  - Archives here: https://sciware.flatironinstitute.org **Check #17!**
  - #sciware Slack channel