MFCF C&O GRAD SESSION
FALL 2023

AGENDA

- Introduction, Help Centre
- Getting online
- Using your desktop machine
  - desktops, accessing your files, central file service, printing, applications
- Academic resources
  - personal web pages using Scholar
  - library journals
- Computing resources
  - Linux environment - servers (fast, big, GPU, HPC), managing jobs and priorities
  - Windows environment - MS Remote Desktop
- Mathematical applications
- Questions

HELP CENTRE

- MC 3017, ext. 46323 (hMFCF) mfcfhelp@uwaterloo.ca
- desktops - re-imaging, downloading software
- personal laptop wired connections - submit RT ticket
- accounts, printing
- Request Tracker - https://rt.uwaterloo.ca/SelfService/Forms/MFCF/
- please feel free to ask us for help!

GETTING CONNECTED

- two-factor authentication - for campus wide services
- on-campus: wireless and wired connections
  - Wired connection -
    - submit request with MAC address, OS, supervisor, room number, expiry date
- off-campus: VPN
  - use https://checkvpn.uwaterloo.ca/ to verify things work
- Microsoft 365 suite - including Teams

VIRTUAL PRIVATE NETWORK

- Allows remote access to all campus network resources
  - e.g. files, remote desktop services
  - all data transferred are encrypted and secure
- Install VPN from IST. This is a one-time install.
  - https://uwaterloo.ca/information-systems-technology/services/virtual-private-network-vpn
    - includes Windows and Mac instructions
  - the client is called Cisco AnyConnect
  - WatIAM credentials to login
  - use https://checkvpn.uwaterloo.ca/ to verify things work

WIRELESS

- Select eduroam from the list of available Wi-Fi networks
- authentication
  - userid@uwaterloo.ca
  - WatIAM password
- Do NOT run your own wifi service. It just interferes with eduroam and makes it worse for everyone!

WIRED

- submit a request in the MFCF RT queue with the following information:
  - operating system
  - room
  - expiry date
  - MAC hardware address
    - https://uwaterloo.ca/math-faculty-computing-facility/services/wired-connections/how-find-mac-hardware-address
  - sponsor/supervisor

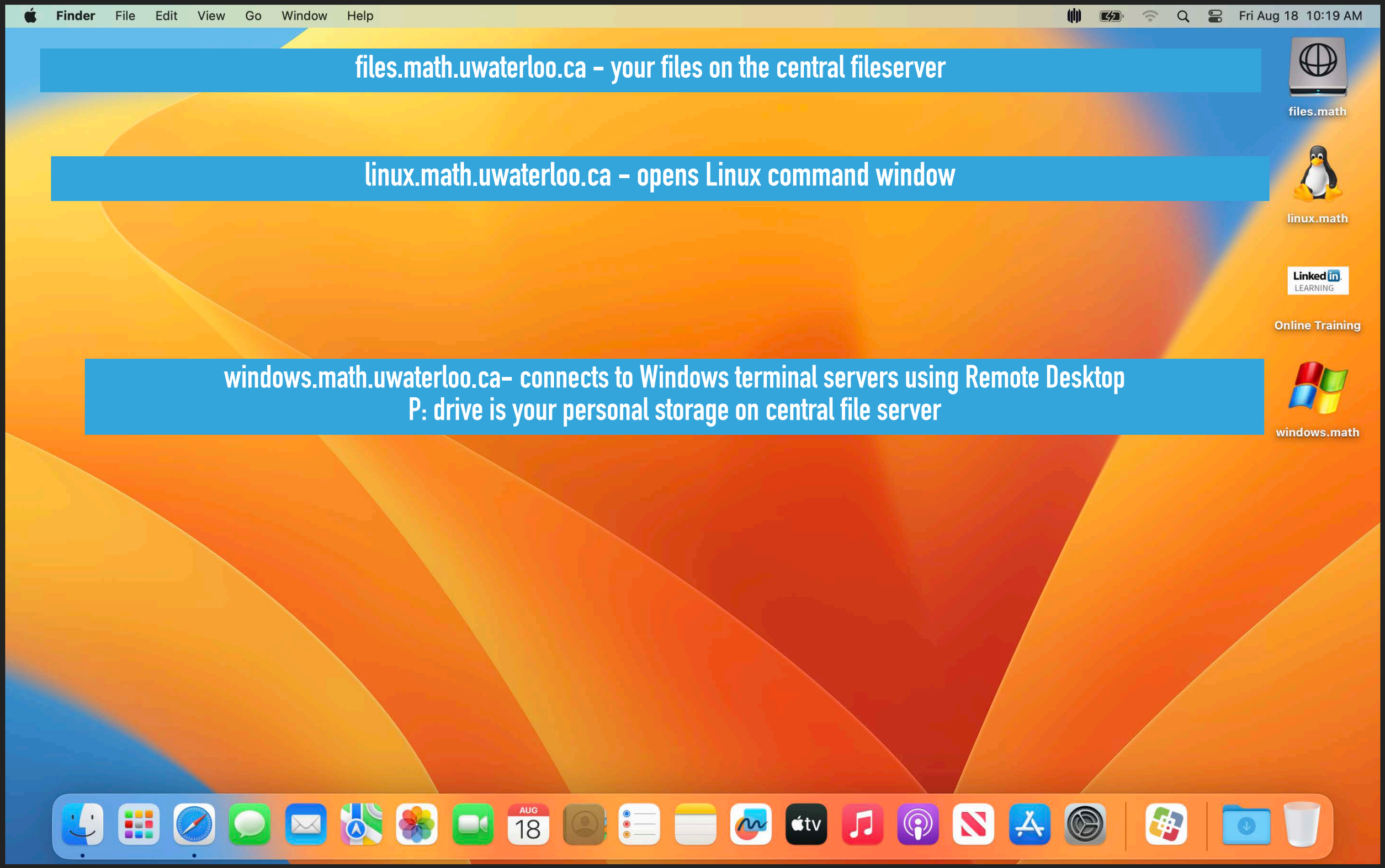
USING YOUR DESKTOP

- desktop machines
- central file service
- printing
- applications

DESKTOPS

- managed by MFCF
  - but you have admin access to install applications
- files on local machine are NOT backed up
  - use the central file server for important files (thesis!)
- Common Mathematical software - Maple, MATLAB, Office suite, R, etc., preinstalled or available via Applications > Self-Serve portal

USING YOUR DESKTOP



DESKTOPS

- Mac minis - icons on the desktop for:
  - files.math.uwaterloo.ca - your files on the central fileserver
  - windows.math.uwaterloo.ca- connects to Windows terminal servers using Remote Desktop
    - P: drive is your personal storage on central file server
  - linux.math.uwaterloo.ca - opens Linux command window
    - more about choice of Linux servers later in the presentation

CENTRAL FILE SERVICE

- central research file server “files.math.uwaterloo.ca"
- central teaching file server - coursework “files.student.math.uwaterloo.ca"
- frequent online backups for safe reliable storage and easy retrieval of old versions
- all central Linux and Windows servers, plus your desktop machines, use the central file servers
- keep your important files there, not on your desktop!

CONNECT TO FILE SERVER FROM YOUR OWN MACHINE

- Use Virtual Private Network (VPN) when accessing campus resources remotely https://vpn.uwaterloo.ca
- store files on the central Math fileserver (back up your data)
  - Mac standalone: Go > Connect to Server…
    - smb://files.math.uwaterloo.ca/UWuserid
  - Windows standalone: Map a network drive
    - \\files.math.uwaterloo.ca\UWuserid
  - Windows Remote Desktop: windows.math.uwaterloo.ca
    - P: drive (files are stored automatically on the file server)
  - Linux: File Manager > Connect to Server…
    - smb://files.math.uwaterloo.ca/UWuserid
    - ssh to linux.math.uwaterloo.ca

PRINTING

- access is automatic once registered - check with admin for location of printers
- for thesis only - do not print books
- can be added to your personal workstation
  - https://uwaterloo.ca/math-faculty-computing-facility/services/service-catalog-printing/adding-printers-your-computer

APPLICATIONS

- math software
  - R, Maple, Julia, Octave (freeware version of MATLAB), Python and many more
  - MATLAB - Free campus wide license. See https://uwaterloo.atlassian.net/wiki/spaces/ISTKB/pages/284525621/Download+or+use+MATLAB+online
  - others at https://uwaterloo.ca/information-systems-technology/services/software-faculty-and-staff/licensed-software-university-waterloo (some free, some paid by your supervisor)
- typesetting
  - LaTeX, including Overleaf Commons (www.overleaf.com/edu/uwaterloo)
- Zoom - Free campus wide license. https://uwaterloo.zoom.us

APPLICATIONS – OVERLEAF

- Overleaf is a collaborative online document editor - understands LaTeX for typesetting math
  - www.overleaf.com/edu/uwaterloo
- works in browser
- templates for UW thesis style, etc.
- UW site licence, free of charge for grad students

APPLICATIONS – ZOOM

- UW site licence free for grad students
- pro/educational level features
- https://uwaterloo.zoom.us
  - click Sign In, use your UWuserid@uwaterloo.ca address and WatIAM password
- https://uwaterloo.atlassian.net/wiki/spaces/ISTSERV/pages/42583425333/Collaboration+-+Zoom
- we use Microsoft Teams a lot here too

ACADEMIC RESOURCES

- personal web sites
  - UW Scholar
- library journals
  - start at uwaterloo.ca/library
  - find articles for your department
  - Math representative

PERSONAL WEB SITES

- UWaterloo Scholar https://uwaterloo.ca/scholar
  - does not require programming or coding skills
  - easy to use tools, self managed with templates/content modules
    - bio, CV, publications, events, etc.…
    - publications can be imported into UWaterloo Scholar
- Documentation and guidelines:
  - https://uwaterloo.ca/web-resources/scholar

- how long to keep Scholar site after leaving:
  - indefinite (cannot edit after you leave though)
    - make sure to put in a link to a new site before it's read only
    - request to have it shut down/hidden

LIBRARY JOURNALS

- start at uwaterloo.ca/library
  - Quick Links -> Get Access From Anywhere to connect using your surname and barcode on back of WatCard
  - Quick Links -> Research Guides
    - scroll down, click Combinatorics & Optimization, then click the title
    - select the “Find Articles” tab for links to various research databases including MathSciNet (on AMS.org site)
    - check out “Links of Interest” tab
- Library support person for Math: Rebecca Hutchinson (r3hutchinson@uwaterloo.ca)
- training workshops may be available, or just email Rebecca with any questions

COMPUTING RESOURCES

- Linux environment
  - servers
  - job management
- Windows environment
  - servers
  - Remote Desktop

LINUX ENVIRONMENT

- Servers
- Job management

SERVERS

- types of Linux servers
  - aliases - ssh to one of: linux.math, biglinux.math, fastlinux.math, and linux.student.math (course work only)
  - GPU servers, Parallel clusters
  - departmental-specific server: pegasus.math.private (by request)
- what they can be used for:
  - Math applications/IDEs
    - MATLAB, SAGE, CPLEX, Maple, R, Julia, NumPy, SciPy, etc.
  - compilers and numerical libraries (gcc, GSL)
  - parallel tools on biglinux (OpenMP) and the clusters (MPI)
    - lots more memory than your supplied desktop or laptop
  - long running jobs

BIGLINUX.MATH

- for large memory or multi-process jobs
- pool of computers with 4 high-core-count CPUs, large memory

FASTLINUX.MATH

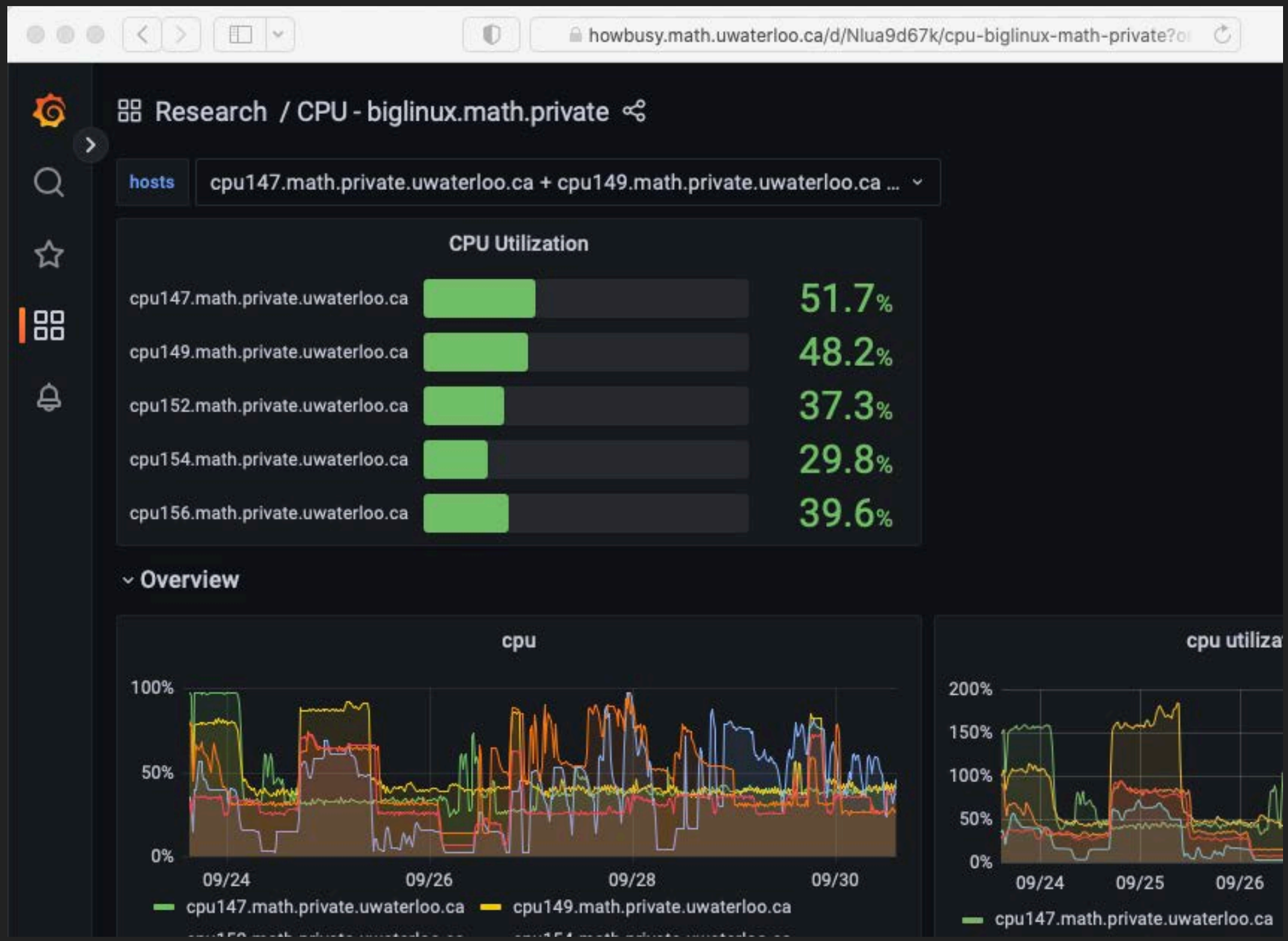
- for jobs where processor speed is most important
- pool of computers with fastest CPUs
- 2 CPUs per machine, low core count; moderate memory

LINUX.MATH

- for light-duty casual use
- pool of older computers

CHOOSING A MACHINE FROM ONE OF THE POOLS

- https://howbusy.math.uwaterloo.ca/



SOFTWARE ENVIRONMENT

- Ubuntu 22.04
- see details at
  - https://uwaterloo.ca/mfcf/services/ -> Computing -> Research and staff Linux servers

JUPYTER

- web-based application that allows you to use or create documents that contain live code, equations, and visualizations
- use it remotely for Python, R, MATLAB, Octave, etc., or a command shell for quick work
- https://jupyter.math.uwaterloo.ca

GPU SERVERS

- gpu-pr1-01.math / gpu-pr1-02.math
- two 14-core CPUs, 128GB RAM / two 32-core CPUs, 1 TB RAM
- four NVIDIA Tesla P100 GPUs / eight A100 GPUs
- CUDA and other parallel GPU tools
- access via SLURM job scheduler – see our web site
  - https://uwaterloo.ca/mfcf/services/specialty-research-linux-servers

PARALLEL CLUSTERS

- mosaic - hybrid, with InfiniBand
  - 19 nodes with 20 cores, 256 GB RAM, and 2 Tesla K20 GPUs
  - four nodes with 32 cores, 768 GB RAM
- Hpc-pr3
  - 8 nodes with 32 cores and 128 GB per node
- access via SLURM job scheduler – see our website
  - https://uwaterloo.ca/mfcf/services/specialty-research-linux-servers

HIGH-PERFORMANCE COMPUTING

- Digital Research Alliance of Canada https://alliancecan.ca/
  - formerly Compute Canada
- graham cluster located here at UW
  - 32,000 CPUs
  - InfiniBand high-speed interconnect
  - 320 NVIDIA P100 GPUs
- sponsored by your faculty member, free of charge

JOB MANAGEMENT

- background jobs
- nice
- nohup, screen, tmux

PUT JOBS IN THE BACKGROUND

- if you do this:
  - $ firefox

you can’t run another command until firefox exits

- put an ampersand on the end:
  - $ firefox &

it runs in the background and you can type more commands

- see what jobs you have in the background:
  - $ jobs
- e.g. bring the third one to the foreground again:
  - $ fg %3
- e.g. kill the second one:
  - $ kill %2

NICE

- commands started at the shell prompt run at normal interactive priority (‘nice’ value of zero)
- having many things competing for interactive priority can make the system feel slow
- so it is not polite (or "nice") to run big/long jobs at normal priority
- use the "nice" command to start a job at a polite background level (value higher than zero):

```
% nice 19 ./a.out &
```

- use the "renice" command to reset the priority of a running job:

```
% ./a.out &
% ps -u
USER       PID %CPU %MEM    VSZ   RSS TTY      STAT START   TIME COMMAND
rblander 14142  0.8  0.0  13796  2016 pts/3    Ss   11:29   0:00 ./a.out

% top
  PID   USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+   COMMAND
14142 rblander  20   0   269m 150m 5092 R 100.0  0.0   0:01.12 ./a.out

% renice 19 14142

% top
  PID   USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+   COMMAND
14142 rblander  39  19   269m 150m 5092 R 100.0  0.0   0:01.23 ./a.out
```

BATCH (OLD ENVIRONMENT ONLY)

- leave a job running after log-out
  - submits job to a queue
  - runs when conditions allow (load, etc.)
  - send you mail about status
  - restarted if interrupted
- syntax: batch queue name -c “command options…”
  - examples:
    - % batch big -c "./my_big_job.a <infile >outfile”
    - % batch long -c “./my_long_job.a <in>out”
    - % batchstatus
    - % batch cancel -q big 1234
  - see “man batch”

NOHUP

- log-out sends “hang up” (HUP) signal to child processes
- “nohup” command blocks HUP signal
- syntax: put ‘nohup’ in front of usual command line
  - % nohup ./myprog.a <infile >outfile
  - % nohup matlab -nojvm -r [a,b,c]=myarray -logfile myarray.log
  - % logout

SCREEN

- lets you disconnect from session and reconnect later
- start: screen
- disconnect: ctrl-A d
- reconnect: screen -x

TMUX

- terminal multiplexer: multiple terminal sessions in one window

LIMIT

- protects against accidental long-running jobs
- default is 1200 seconds (20 minutes) CPU time
- Increase it in your shell control file
  - open the .cshrc file with your favourite editor
    - e.g. change “limit cputime unlimited”
    - e.g. change “limit memoryuse unlimited”
- log out and log back in again for it to take effect
- “man limit”

WINDOWS ENVIRONMENT

- Servers
- Remote Desktop

SERVERS

- types of Windows servers
  - windows.math
    - pool of servers for research computing
    - P: drive is files.math
  - wingpu.math
    - GPU server with three NVIDIA T4 GPUs
  - windows.student.math
    - pool of servers for student/coursework computing, NOT for research
    - M: drive is files.student.math

REMOTE DESKTOP

- Microsoft Remote Desktop
  - icon on Mac mini desktop
    - can disconnect from a session and reconnect later
      - but on windows.student.math, disconnected sessions get closed after two hours
- save your work often
- write code with checkpoint methods

WEB RESOURCES

Math Faculty Computing Facility (MFCF) »

Mathematical Applications

Maple worksheets - developed for Applied Math courses

MATLAB tutorials

Introduction to GPU computing in MATLAB, R, and C++ with CUDA (PDF)

R and GPU computing- specifically for Statisticians (PDF)

Comparison of R and Python Data Science Applications

Scientific Blogging with R and Blogdown

Dedalus

MFCF Help Centre Information

EMAIL, LEARN, QUEST AND MORE FROM

IST SERVICES

WEB RESOURCES

- MFCF Web site - uwaterloo.ca/mfcf
- LinkedIn Learning (LiL)- online training
  - formerly known as Lynda.com
- Request Tracker - online reporting system
- handy one-page reference to all the main topics we covered:
  - https://uwaterloo.ca/mfcf/mfcf-information-sheet-math-faculty
- services for grad students:
  - https://uwaterloo.ca/mfcf/services/audience/25

THANK YOU

From the MFCF Team

suggestions for future topics?

https://uwaterloo.ca/math-faculty-computing-facility/services/audience/25