



MFCF APPLIED MATH GRAD SESSION FALL 2024

AGENDA

- ▶ Introduction, Help Centre
- ▶ Getting online
- ▶ Using your computer
 - ▶ 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, name of 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 Secure Client
 - ▶ WatIAM credentials to login

WIRELESS

- ▶ Select eduroam from the list of available Wi-Fi networks
- ▶ authentication
 - ▶ [userid@uwaterloo.ca](mailto:user@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>
 - ▶ name of sponsor/supervisor

USING YOUR COMPUTER

- ▶ desktop
- ▶ central file service
- ▶ printing
- ▶ applications

DESKTOPS

- ▶ managed by MFCF
 - ▶ but you can request 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

files.math.uwaterloo.ca – your files on the central fileserver

linux.math.uwaterloo.ca – opens Linux command window

windows.math.uwaterloo.ca – connects to Windows terminal servers using Remote Desktop
P: drive is your personal storage on central file server



files.math



linux.math



Online Training



windows.math



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-catalogue-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)
 - ▶ make sure to put in a link to a new site before it's read only
 - ▶ request IST 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 Applied Math, 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
- ▶ Loaner laptops - high end Windows, Mac, and Linux
 - ▶ laptops with GPU for highly parallel computing
 - ▶ can be borrowed short-term with authorization from supervisor

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 servers: Fluids group, Control group , Bauch Lab, etc.
 - ▶ ask your supervisor if they have extra resources for you to use and if so, they can submit a [request](#) to us
- ▶ 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 and processors 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/> -> Research 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 / gpu-pr1-02 / gpu-pr1-03 / gpu-pr1-04
- ▶ NVIDIA P100, A100, H100, and L40S
- ▶ 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

- ▶ 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

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

WINDOWS ENVIRONMENT

- ▶ Servers
- ▶ Remote Desktop

SERVERS

- ▶ types of Windows servers
- ▶ file storage is mapped to P: drive (files.math)
 - ▶ windows.math
 - ▶ pool of servers for research computing
 - ▶ wingpu.math (request access)
 - ▶ GPU server with three NVIDIA T4 GPUs
 - ▶ mondo.math (request access)
 - ▶ GPU workstation for highly parallel computing
 - ▶ windows.student.math
 - ▶ pool of servers for student/coursework computing, NOT for research
 - ▶ M: drive (files.student.math)

REMOTE DESKTOP

- ▶ Microsoft Remote 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

Mathematical Applications

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[Maple worksheets](#) - developed for Applied Math courses

[MATLAB tutorials](#)

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

[Accelerating MATLAB code with GPUs](#) - compares CPU and GPU performance

[Accelerating physics calculations with CUDA in Python using Numba: A Monte-Carlo example](#)

[Theoretical Background Notes for "Accelerating physics calculations with CUDA in Python using Numba"](#)

[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>