Linux, command line & MetaCentrum Use of Linux command line not only for CESNET's MetaCentrum

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January 14 to 16, 2025



Outline I

Introduction Learning machine What it is a "UNIX" Licenses and money

Linux

Generally about Linux Choose one Differences

3 UN*X

Disks and file systems Types of users Directory structure Files and directories Permissions

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Introduction	Linux	UN*X	Command line	Text	Scripting	Software	MetaCentrum	Git	Administration	The End
Outline	II									
Text										

4	Command	line	

BASH and other shells ("command lines")

Screen

SSH - secure shell and screen

BASH

Directories

Archives

Searching

Globbing, wildcards, quotes

Variables

Input, output and their redirecting Information and processes

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Outline III

Network Parallelization Timing

5 Text

Reading Extractions AWK Manipulations Compressed text Comparisons Editors Regular expressions

6 Scripting

 Scripting
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Introduction Linux UN*X Command line Text Scripting Software MetaCentrum Git Administration The End

Outline IV

Basic skeleton BASH variables Functions Reading variables Branching the code Loops

7 Software

- Packages Compilation Java Windows applications Scientific applications
 - Games

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Introduction						
Outline	V					

MetaCentrum

 Information
 Usage
 Tasks
 Graphical connection
 More services

9 Git

Git principle Git basics

AdministrationSystem services

🕦 The End

Resources

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The very end

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Introduction

First steps in the world of Linux and open-source software

1 Introduction

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The course information

- The course page: https://trapa.cz/en/course-linux-command-line-2025
 Česky: https://trapa.cz/cs/kurz-prikazove-radky-linuxu-2025
- Subject in SIS: https://is.cuni.cz/studium/eng/predmety/index. php?do=predmet&kod=MB120C23
 - Česky: https://is.cuni.cz/studium/predmety/index.php?do= predmet&kod=MB120C23
 - For students having subscribed the subject, requirements are on next slide
- Working version of the presentation is available at https://github.com/V-Z/ course-linux-command-line-bash-scripting-metacentrum - feel free to contribute, request new parts or report bugs

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Requirements to exam ("zápočet")

- 1 Be present whole course.
- 2 Be active ask and answer questions.
- Write short script solving any task the student is (going to be) solving. E.g. prepare script to process student's data on MetaCentrum. Or short script to do anything the student needs to do. This will be very individual. According to topics and interests of every student. Students can of course discuss with anyone, use Internet, manuals, etc. The aim is to learn how to solve real problem the student has/is going to have.
- Write at least one page (can be split into multiple articles) on Wikipedia about any topic discussed during the course. Again, this is very open, students can write about any topic they like. I prefer native language of the student (typically to make larger non-English Wikipedia).

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Materials to help you...

- Download the presentation from https://soubory.trapa.cz/linuxcourse/ linux_bash_metacentrum_course.pdf
- Download the scripts and toy data from https://soubory.trapa.cz/linuxcourse/scripts_data.zip
 - Note: Open the scripts in some good text editor (slide 159) showing syntax highlight, line numbers, etc. (NO Windows notepad); the files are in UTF-8 encoding and with UNIX end of lines (slide 76; so that too silly programs like Windows notepad won't be able to open them correctly)
 - Never ever open any script file in software like MS Word they destroy quotation marks and other things by "typographical enhancements" making the script unusable

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Virtual machine for learning

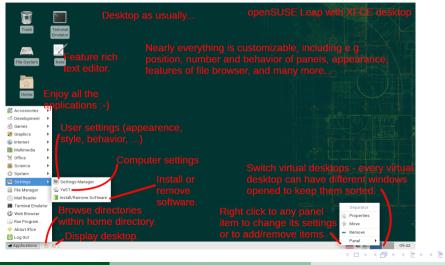
- If you do not have Linux installed, download and install VirtualBox from https://www.virtualbox.org/
- Download openSUSE Leap 15.6 Linux distribution for this course from https://botany.natur.cuni. cz/zeisek/openSUSE_Leap_ courses.ova (~8.2 GB)
- Launch VirtualBox and go to menu File | Import appliance... to import it. When done, launch it (Start)
- See also https://trapa.cz/en/ vm-for-courses



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Enjoy learning virtual machine for the course



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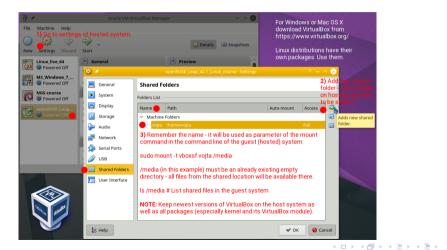
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VirtualBox shared folder I

VirtualBox can be configured to share folder with host operating system



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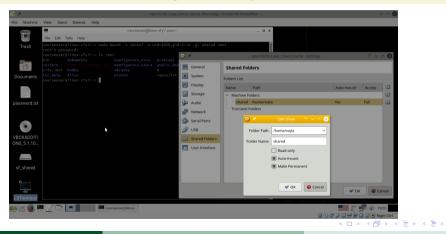
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VirtualBox shared folder II

Go to menu "Devices | Shared Folders" and set pair of folders

sudo mount -t vboxsf -o uid=\$UID,gid=\$(id -g) shared /mnt



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What it is UNIX, Linux and GNU I

- UNIX
 - Originally developed in Bell labs of AT&T in 1969, written in C, since then rich evolution...
 - Trademark only systems passing certain conditions (paid certification) can be called "UNIX" — Solaris, HP-UX, AIX, etc. (commercial systems for big servers; nowadays rare)
 - **Main principles:** simple, multitasking, hierarchical structure, network, for more users (takes care about permissions etc.), configuration written in plain text files, important relationships among applications (generally one application = one task they are chained), work primarily with text, has kernel and API (interface to communicate with the rest of the system)
- UNIX-like (UN*X, *nix)
 - Systems compatible with UNIX (Linux, BSD and its variants, macOS, ...)
 - Mainly open-source (UNIX is commonly commercial source code is not publicly available, but its specification is)
 - Nowadays prevailing over "old" UNIX systems, used in many devices from tiny embedded toys to huge data centers
 - Try to provide same quality as paid systems, but (mostly) for free

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What it is UNIX, Linux and GNU II

 Many courts about copyrights, parts of code, patents (USA allow software patents, EU not) — GNU, Linux, BSD, etc. try to ensure to have only code not covered by any patents to avoid possible legal issues

• GNU

- "GNU's Not Unix!" but it is compatible, respects its principles
- System written from scratch, following ideas of UNIX
- Since 1984 Richard Stallman (founder of Free Software Foundation) tried to make new kernel (Hurd not finished yet...)
- Generally set of basic system tools working with many kernels (Linux, BSD*, macOS, ...), also present in many commercial paid UNIX systems
- Source code is free and open anyone can study it (Security!), report bugs, contribute, modify, share it, get inspiration, ...
- GNU General Public License (GPL) free spirit of open-source license, idea, how to share software to benefit everyone

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What it is UNIX, Linux and GNU III

- Inspired open public software development crucial for our usage of Linux & al.
- Linux
 - First version of kernel (core of the system) written by Linus Torvalds in Helsinki in 1991
 - Kernel was in principle inspired by various UNIX systems and using GNU tools for standard work
 - Quickly became popular anyone can take it and use for any needs, adopt (modify it), etc.
 - Used in small embedded (commonly network) devices, mobile devices (book readers, Android, ...), personal computers, servers (from home level to biggest data centers), ...
 - Nowadays powering most of the Internet
 - Anyone can contribute not only code, also documentation, design, translations, ...
 - Most of people working with UNIX are using Linux (or macOS)
 - Powering everything from little IoT toys and devices to 100% of top 500 supercomputers
- GNU tools and Linux kernel are two important (but not sole) pieces of building set forming modern operating system "Linux distribution"

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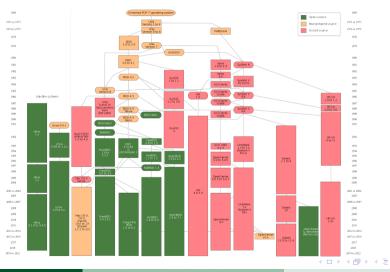
What it is UNIX, Linux and GNU IV

- "Linux" nowadays usually mean Linux kernel + GNU basic tools (thus correctly "GNU/Linux") + thousands of various another applications (= "Linux distribution") ecosystem of (free) open-source GNU/Linux applications of various origin forming together what we usually call simply "Linux"
- Term "Linux" has various meaning (see further)
 - If we mean only Linux kernel or whole distribution
 - If we talk about little embed Internet of Things (IoT) device, some mobile device, personal computer, server, supercomputer, ...
 - We can talk about particular Linux distribution (see further)/use case, or generally...

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Extremely simplified UNIX phylogeny



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Most common UNIX-based systems (except Linux)

- Apple macOS (previously Mac OS X) system kernel is based on older BSD and uses plenty of GNU tools (although mostly older outdated versions)
- BSD one of the oldest operating systems, still developed in many independent variants
 - Still very popular especially on servers, for special purposes, etc.
 - License allows closing of the code used by Apple macOS kernel, PlayStation firmware, ...
 - Installation and management is for beginners usually harder than Linux, everything must be done manually, not so common as Linux anymore
 - E.g. FreeBSD, DragonFly BSD, OpenBSD, TrueNAS (for storage servers), ...
- Solaris commercial, not very common anymore
 - Mainly special servers, paid
 - Several community-based variants freely available
- Command line usage is nearly same across UN*X systems all follow same standards, use more or less same set of tools

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Cathedral vs. market place

What is principal difference between free open-source and commercial software

- Commercial software is like a cathedral
 - Pay big money and get it in the state which the architect like
 - User can not modify it (or it is terribly expensive)
 - Might be you don't need everything but still paying whole set
- Free open-source software (FOSS) is like a market place
 - Find there many producers of same tools pick up those you like freedom of choice
 - Take exactly the tools you need any combination is possible
 - Much cheaper to shop there
- Both have pros and cons depends what you wish...
- Consider e.g. difference between usage of full-featured and expensive Geneious (theoretically everything you need to process genetic data) vs. searching for hundreds of free tools and pipelines on the Internet (GitHub, R packages, fora, ...)
- According to book by Eric S. Raymond

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Free and open-source software - (F)OSS I

- Free like freedom of speech, not like free beer!
- Open-source source code can be seen by the holder of the license (not necessary by everyone can be paid)
- Not every OSS (generally less strict conditions) has to be FOSS (you can do with it (almost) whatever you like) source code might be available under some circumstance (only to look), but modification and/or reuse of the code prohibited (and then it is not **free**)
- GNU GPL ("copyleft") probably most common OSS license, strict, viral derived code has to keep the license surprisingly not fully "free" as it doesn't allow changes of license
- LGPL Lesser GPL more permissive
- BSD license permissive allow derived code to became closed-source (commonly used by e.g. Apple macOS, Safari browser, small electronics, ...)
- Apache or Mozilla licenses etc. specific use in particular software

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Free and open-source software - (F)OSS II

- Creative Commons (CC) software licenses are not suitable for multimedia, text, etc. CC has many options (including denial of reuse of the product), see https://creativecommons.org/
- And many more licenses...

Spirit of FOSS

- Orientation might be tricky, but practical output for users is same the software can be independently checked for bugs, backdoor, malware, can be improved and under some circumstances, new software can be derived, and usually, it is available for free
- Aim is to "liberate" software to keep open sharing of ideas, mutual improve and security control
 - Although the point is clear, there are debates how to reach it...

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Free and open-source software - (F)OSS III

- Practical output of using open-source licenses for the user
 - Software can be used anywhere
 - Software can be modified including various fixes of older code to work properly, or for different systems (author worked e.g. on Linux and someone else will do version for macOS or Windows)
 - User can learn from the software (from the code), new software can be developed on top of it
 - Easier to find and trace bugs
 - Security no backdoors, possibility to do various audits, screenings, etc.
 - Bugs (problems) in the code can fixed by nearly anyone
 - Often available for free (e.g. on services like GitHub or SourceForge)
 - Easier distribution of the software (can be copied into various repositories, like those of Linux distributions, Conda or Homebrew)

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How to make money with free open-source software?

- Traditional model user rents right ("buys a license") to use the software (and sometimes for support usually for extra money)
- Common mistake software is not "bought" only license is rented ("permission to use it" with many limitations)
- Software as service
 - (F)OSS is available for free user can use it as it is or buy a support help of any type
 - No vendor lock-in user has the code, so he can modify the software himself, change provider of the services, ...
 - Cheap for user as well as company company specialized for one task, let's say server database, doesn't have to take care about the rest of the system someone else does; user pays only what he needs
 - E.g. anyone can download and install Content management system like Drupal or WordPress on their server to create custom web page, or there are plenty of companies providing service of hosting such system on their server, including various user support, and in case of need it is easy to change such provider

Generally about Linu	ĸ	Choose on	е	Differ	ences		

Linux Generally about Linux

Linux

Generally about Linux Choose one Differences

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Generally about Linux		Choose on	e	Differe	ences		

What it is a "Linux"

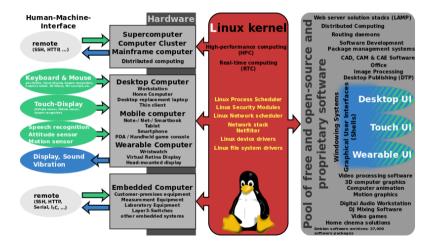
- Operating system respecting principles of UNIX
- Components
 - Linux **kernel** basic part of the system responsible for hardware and very basic low-level running of the system ("Linux *sensu stricto*")
 - GNU core utilities basic applications
 - Graphical user environment (GUI) many choices
 - Many other applications according to use whatever imaginable

• Linux distribution ("Linux sensu lato")

- Somehow assemble Linux kernel, basic tools and some applications
- Optionally add some patches and extra tools and gadgets
- Make your own design! (very important;-)
- If lazy, remake existing distribution (using e.g. web service)
- Still surprised there are hundreds of them?
- It is like Lego pieces are more or less same across distributions, but result is very variable
- From "general" for daily use (pick up whatever you like) to very specialized special hardware devices, network services, rescue, ...

Introduction							
Generally about Linu	x	Choose one	е	Differe	ences		

Linux kernel and other parts around it



https://en.wikipedia.org/wiki/Linux_distribution

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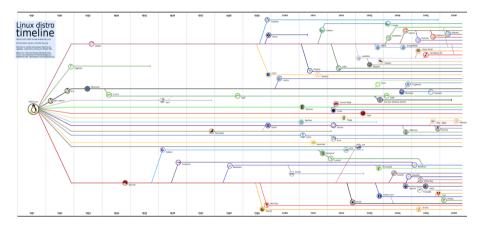
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Generally about Linu	x	Choose on	ie	Differe	ences		

Extremely simplified adaptive radiation of Linux distributions



https://en.wikipedia.org/wiki/List_of_Linux_distributions and https://distrowatch.com/ (~900 distributions, ~250 active)

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Generally about Linux		Choose on	e	Differe	ences		

Most common Linux distributions

- Debian (DEB) based
 - Debian one of oldest and most common, especially on servers
 - Ubuntu (nowadays probably the most popular on PCs and notebooks) and derivatives Kubuntu, Xubuntu, Lubuntu, ... (according to GUI used most of the system is same)
 - Mint Based on Ubuntu as well as Debian, user-friendly, popular
 - Kali, KNOPPIX, elementaryOS, Pop!_OS, MX Linux, Zorin OS, ...
- Red Hat (RPM) based
 - Red Hat probably the most common commercial
 - Fedora "playground" for Red Hat very experimental
 - Centos Clone of Red Hat
 - openSUSE SUSE is second largest Linux company, openSUSE is community distribution (free) companion of SUSE Linux Enterprise
 - Mageia, PCLinuxOS, ...
- Manjaro, Solus, ...
- Android (practically Linux kernel, touch interface & Java)
- For experienced users: Arch, Slackware, Gentoo, ...

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Generally about Linux	ĸ	Choose one	e	Differ	ences		

Graphical User Interfaces (GUI)

More like "Mac-style", "Windows-style" or something else? Feature rich or minimalistic?

- Most of GUIs are available for most of common distributions one is picked as default and "only" color style is different
- KDE one of the most common, feature extremely rich, basically "Windows-like" (can be changed), extremely versatile
- GNOME one of the most common, relatively simplistic interface, but still feature rich, "Mac-like"
- XFCE lightweight version of older GNOME for older computers or users not willing to be disturbed by graphical effects, basically "Mac-like" looking, but panels can be moved to "Windows style"
- Cinnamon remake of GNOME to look more like Windows...
- Unity originally developed by Ubuntu (discontinued, now community based), "Mac-style"
- And much more...
- Choose what you like doesn't matter much which one...

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Ubuntu with GNOME



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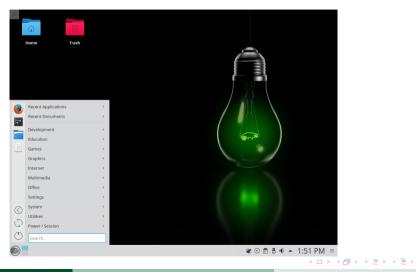
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openSUSE with KDE - Kubuntu is same, but blue...



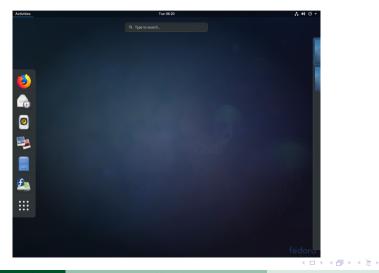
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Fedora with GNOME – GNOME is always almost same



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Linux Mint with Cinnamon



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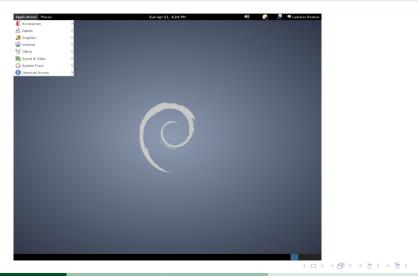
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Generally about Linux		Choose on	e	Differe	ences		

Debian with XFCE - Xubuntu has more "modern" design



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XFCE in Xubuntu, openSUSE, Fedora and Linux Mint



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Introduction							
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Dolphin (KDE file manager) — default for openSUSE (inset) and after tuning in the same distribution...

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Introduction								
Generally about Lin	ux		Choose or	e	Differe	ences		
How to t	try Li	nux?	I					

- If unsure what to do, ask someone for help. ;-)
- Install it on some computer together with or instead of Windows
 - If you can use whole disk, just boot from CD/USB and click "Next" ...
 - If you don't have whole disk, you need at least one (commonly more) disk partition(s) if you don't know how to manage them, ask someone skilled...
 - Major updates of Windows 10/11 or Windows reinstall use to destroy bootloader and it is not possible to start Linux anymore (although it can be usually easily fixed)
- Live CD/USB
 - The most easy burn ISO image of CD from web of almost any Linux distribution or use for example UNetbootin to prepare bootable flash
 - You only have to know how to boot from CD/USB (usually press ESC, DEL, F2, F10, F12, ... when starting computer varies according to manufacturer)
 - Commonly done to rescue data from broken Windows installations... ;-)
- Virtualization (slide 12)
 - Requires powerful computer Intel i7 or AMD Ryzen, over 12 GB of RAM and hundreds of GB

Generally about Linu	x	Choose one	e	Differe	ences		

How to try Linux? II

- Install virtual machine (probably the most easy is VirtualBox) allows install and run another operating system inside host as an ordinary application very easy and comfortable
- Linux subsystem in MS Windows Store (Windows 10 and 11)
 - To install follow https://learn.microsoft.com/windows/wsl/about
 - Version 1 only for command-line applications (it has some problems with paths, text files, ...)
 - Version 2 works well for most of tasks and allows GUI (experimental)
- Cygwin
 - Download and install from https://www.cygwin.com/
 - It is not native Linux, it is collection of GNU and open-source utilities compiled to work on Windows as more or less standard Windows applications
 - Follows POSIX standards (i.e. it works like normal UNIX command line, with all features)
 - Every application must be specially compiled to be able to work under Cygwin (it is sometimes complicated)
 - Collection is large, include also GUI and DE, but not everything is easy working
 - Installation of custom software might be very hard...

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Introduction								
Generally about Linu	X		Choose on	е	Differe	ences		
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The Linu	x div	/ersity	′ 					

- Try several distributions and just choose one you like...
- If selecting among the most common, it doesn't matter much which one you pick up
- Which design do you like?
- Which distribution is your friend or colleague using? To have someone to ask for help...
- You can change GUI (or its design) without change of distribution, it use to be highly configurable
- Applications are still same no difference in Firefox across distributions keep your settings when changing distribution
- Everyone using Android is using Linux install some terminal emulator there :-)
- Special use TrueNAS for home as well as business file servers, Parted Magic and/or SystemRescue to repair broken system (disk failure) and save data, ...

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Generally about Linux		Choose one	е	Differe	ences		

Differences among (common) Linux distributions

- Design and colors ;-)
- Default GUI (others can be installed)
- Applications available right after installation
- Default settings (not much)
- Package management especially in command line
- Development model conservative or experimental, fast or slow
- Management of system services (how to start/stop certain services like database or web server) not important for daily usage for most of users
- Sometimes in location of some system files (can be customized) also not important in daily usage of most of users
- Kernel is almost same, applications are same and used in same way...
- Command line is almost same across Linux, and almost same as in other UNIX systems (macOS, ...)

Disks and file system:	5	Types of u	sers Dire	ectory struc	ture	Files and direc	tories	Permissions	Text	

UN*X

Theory and principles of UNIX-based operating systems

3 UN*X

Disks and file systems Types of users Directory structure Files and directories Permissions Text

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Vojtěch Zeisek (https://trapa.cz/)	Linux, command line & MetaCentrum	January 14 to 16, 2025	44/317

Disks and file system	5	Types of us	ers Dire	ctory struc	ture	Files and direc	tories	Permissions	Text	

Short overview of hard disk layout

- Physical disk (piece of hardware) has at least 1 partition division seen in Windows as "disks" (C, D, ...) and mounted directory in UNIX
- MBR older description of disk division, up to 4 primary partitions (OS typically requires at least one to run), one can be extended and contain more partitions, disks up to 2 TB
- GPT newer, no relevant limits, requires UEFI (replacement of BIOS responsible of start of nowadays computers)
- If unsure what to do, high probability to break it ...
- Blank new partition has to be formatted to desired file system according to use and target operating system
- Linux distributions have easy graphical tools to manage disk partitions (e.g. GParted)
- Always have backup before such management!

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Disks and file systems	Types of use	rs Dire	ctory struc	ture	Files and direct	tories	Permissions	Text	

Comparison of file systems (limits and compatibility)

FS name	Name length	Signs in name	Path length	File size	Partition size	Supported systems
FAT32	255	Unicode	No limit defined	4 GiB	2 TiB	Any
exFAT	255	?	No limit defined		64 ZiB	Any
NTFS	255	Variable	Variable	16 TiB	16 EiB	Windows (UN*X)
HFS+	255	Unicode Unlimited		8 EiB	8 EiB	macOS
ext4	255	Any, not 🖊	No limit defined	16 TiB	1 EiB	Linux (UN*X)
XFS	255	Any	No limit defined	9 EiB	9 EiB	Linux (UN*X)
Btrfs	255	Any	No limit defined	16 EiB	16 EiB	Linux (only?)
ZFS	255	Unicode	icode No limit defined		256 ZiB	UN*X

- FAT32 (including extensions) is old-fashioned and not reliable FS, but still common in various flash disks and memory cards
- NTFS (basic Windows FS) and FAT do not support UNIX permissions, so they can't be used as system partition in Linux; see also full comparison
- Btrfs, ext4, XFS and ZFS are not accessible from Windows at all (Linux mainly uses ext4)
- Btrfs and ZFS are the most advanced FS in common use

Vojtěch Zeisek

Linux, command line & MetaCentrum

January 14 to 16, 2025

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Disks and file system	s	Types of us	sers Din	ectory struc	ture	Files and direc	tories	Permissions	Text	

Mounting and unmounting disks and removable media

- · Mounting and unmounting of devices require root privileges
- In modern desktop Linux distributions, mounting is done automatically and media are visible mostly in /media or /run/media (and show some icon, widget or so in desktop environment)
- In Linux, physical disks are named from sda to sdz, each disk has partitions (at least one) numbered from 1, (sda1, sda2, sdb1, ...), all are in /dev (/dev/sdc3)
- i eject # Open CD/DVD drive
- ² mount # Which FS (disk partitions) are mounted
- 3 findmnt # See mounted devices in tree-like structure
- 4 mkdir /mnt/point # Empty directory must exist prior mounting into it
- 5 # mount usually recognize FS of mounted device, if not, add '-t FS_type'
- 6 mount /dev/sdXY /mount/directory # Mount disk sdXY to /mount/directory
- 7 mount -t iso9660 -o loop file.iso /mnt/iso # Mount CD/DVD ISO file
- 8 umount /dev/sdXY # Unmount disk sdXY, alternatively use below command
 umount /dev/sdXY # Unmount disk sdXY, alternatively use below command
- 9 umount /mount/directory # Unmount disk from /mount/directory

Disks and file systems	Types of u	sers Dire	ctory struc	ture	Files and direc	tories	Permissions	Text	

Creation and control of FS I

\$ sudo fdisk -l [sudo] password for root:	@ 🔤		/d	ev/sda - GParted		
Disk /dev/sda: 894.26 GiB, 960197124096 bytes, 1875385008 sectors Disk model: Corsair Force LE	<u>G</u> Parted <u>E</u> dit	⊻iew <u>D</u> evice	Partition <u>H</u> elp			
Disk model: Colsai Folce LE Units: sectors of 1 × 512 = 512 bytes Sector size (logical/physical): 512 bytes / 512 bytes I/O size (minimu/potimal): 512 bytes / 512 bytes	New Delete	Resize/Move	Copy Paste	物 🚽 Undo Apply		☑ /dev/sda (60.00 GiB) ▼
Disklabel type: gpt Disk identifier: 55C22C41-DBE7-4E05-8139-FC47E5E342F4 Device Start End Sectors Size Type			v/sda2 11 GiB		/dev/s 24.79	
/dev/sda1 2048 819199 817152 399M Microsoft basic data /dev/sda2 819200 1124351 305152 149M EFI System		1.	1			
/dev/sda2 819200 1124351 505152 1494 Eri System /dev/sda3 1124352 1875384319 1874259968 893.76 Linux LVM	Partition	File System	Label	Size	Used	Unused Flags
	/dev/sda1	ntfs	System Reserved		24.14 MiB	75.86 MiB boot
Disk /dev/mapper/cr_ata-Corsair_Force_LE_SSD_16298021000105550200-part3:		ntfs		33.11 GiB	8.89 GiB	24.22 GiB
Units: sectors of 1 * 512 = 512 bytes Sector size (logical/physical): 512 bytes / 512 bytes	✓ /dev/sda3	extended		26.79 GiB		
I/O size (minimum/optimal): 512 bytes / 512 bytes	/dev/sda5			24.79 GiB	3.39 GiB	21.41 GiB
	/dev/sda6	linux-swap		2.00 GiB		
Disk /dev/mapper/pocitac-odkladiste: 8.72 GiB, 9349103616 bytes, 1825996	8 sectors unallocated	unallocate	b	1.00 MiB		
Units: sectors of 1 * 512 = 512 bytes Sector size (logical/physical): 512 bytes / 512 bytes						
I/O size (minimum/optimal): 512 bytes / 512 bytes						
Disk /dev/mapper/pocitac-korinek: 885 GiB, 950261514240 bytes, 185597952	0 sectors					
Units: sectors of 1 * 512 = 512 bytes Sector size (logical/physical): 512 bytes / 512 bytes						
I/O size (minimum/optimal): 512 bytes / 512 bytes						
Disk /dev/sdb: 931.53 GiB, 1000204886016 bytes, 1953525168 sectors	0 operations pe	inding				11

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Disks and file systems	5	Types of use	ers Dire	ctory struc	ture	Files and direc	tories	Permissions	Text	

Creation and control of FS II

- Work in command line or use graphical tool like GParted...
- All commands require root privileges (slide 54)
- fdisk -1 lists disks and partitions
- To manage disk partitioning use fdisk /dev/sdX or gdisk /dev/sdX
- When hard drive is partitioned, partitions must be formatted in next step
- Commands mkfs.* create various FS, common syntax is mkfs.XXX -parameters /dev/sdXY, where sdXY is particular disk partition
- Parameters can set label and various settings of behavior of the disk partition, check man mkfs.XXX
- To check FS for errors use **fsck**.XXX /dev/sdXY (according to respective FS)
 - The filesystem must be unmounted when checking it
 - XFS uses xfs_repair /dev/sdXY

Disks and file system	S	Types of us	sers Dire	ctory struc	ture	Files and direc	tories	Permissions	Text	

Creation and control of FS III

- Btrfs uses btrfs check /dev/sdXY, if it is unmountable, btrfs-zero-log /dev/XY use to help, last instance is btrfs check --repair /dev/sdXY (dangerous operation)
- If Btrfs is mountable, but there are various FS errors and/or performance issues, btrfs scrub start -Bdf /mount/point, btrfs filesystem defragment -r -v /mount/point and btrfs balance start -v /mount/point — manual running can take long time and strongly slow down the computer
- **tune2fs -parameters** /**dev**/**sdXY** can set various parameters to influence behavior of disk (labels and more) partition
- hdparm -parameters /dev/sdX can set advanced hardware parameters of hard drive

Disks and file systems	Types of us	sers Dir	ectory struc	ture	Files and direc	tories	Permissions	Text	

Creation and control of FS IV

- The most convenient is using graphical tools available in all distributions...
 - In openSUSE there is YaST administrative module from command line launch yast --qt partitioner for graphical or yast disk for text-based version
 - All distributions have graphical tools like GParted where it is possible to comfortable manage disks
- df -h shows available/occupied space on disks/partitions, but because of special features of Btrfs it doesn't show every time correct values for this FS it is better to use btrfs filesystem df /mount/point (/mount/point use to be the most commonly /)
- On UNIX FS, defragmentation and another maintenance tasks use to be done in background when computer is idling unless there is at least ~20% of free space on the device, this is not any problem and there are no performance issues
- Users must be sure what they are doing, otherwise system can be damaged

Disks and file system	s	Types of us	sers Dire	ctory struc	ture	Files and direc	tories	Permissions	Text	

Another manipulations and information

- dd is powerful, but potentially dangerous tool used to backup or write disks or partitions (commonly to create bootable USB media)
- If writing disk image to the disk (sdX), disk's partition table is discarded and the disk is covered by whatever is in the ISO image
- dmesg # Recent entries in main system log filter with grep, tail, ... dmesg | grep sd | tail # Get information about recently plugged media # dd produces physical copy of whole device - including empty space d dif=/dev/sdX of=image.iso # Backups disk sdXY to imago.iso 5 dd if=image.iso of=/dev/sdX # Used to write e.g. image of Linux live # media to USB flash disk (Check sdX!) 1 nav # Comfortably browse recent logs, quit by "q"
 - If there are encrypted partitions, they are in /dev/mapper/...
 - If LVM (slide 53) is used, see **1vscan** and **pvscan** to find correct location in /dev/
 - Disks are also accessible through /dev/disk/by-<TAB><TAB>

Disks and file system	s	Types of us	sers Dire	ctory struc	ture	Files and direc	tories	Permissions	Text	

Put together more disks

Extend space and get higher data security

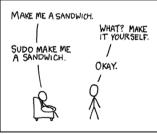
- RAID Redundant Array of Inexpensive/Independent Disks
- RAID 0 stripping, no redundancy, no security, speed up (two or more disks joined into one, files divided among disks)
- RAID 1 mirroring even number of disks of same size resulting capacity is half, very fast, secure
- RAID 5 at least three disks, one is used for parity control (in RAID 6 two disks are used for parity control), little bit slower, popular in cheaper storage servers (NAS)
- Combinations (RAID 10, ...)
- LVM Logical Volume Management built over several partitions/disks seen by OS as one continuous space, can be dynamically managed
- Functionality of RAID and LVM (and more) is more or less covered by Btrfs and ZFS

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Disks and file systems	Types of u	sers D	irectory stru	cture	Files and dired	ctories	Permissions	Text	

Root vs. "normal" user

- Root is administrator more than God (of the server) can do anything
- Other users have limited permissions
 - System users providing particular service (web server, database, networking service) are as restricted as possible to do the task security
 - "Human" users don't have access to system files (at least not for modification), homes of users are separated



https://xkcd.com/149/

Disks and file systems	Types of users	Direc	ctory struc	cture	Files and direc	tories	Permissions	Text	

Becoming root

- Root privileges are required for any administrative task (install of software package, change of system settings, ...)
- Word "root" is used as name for system administrator user, and also for top of filesystem directory hierarchy (/)

```
# Gain root privileges
<sup>2</sup> su # Requires root password (stay in current directory)
3 su - # Requires root password (go to /root)
4 su -c "some command" # Launch one command with root permissions
<sup>5</sup> su USER # Became USER (USER's password is required)
<sup>6</sup> sudo -i # For trusted users, became root (asks for user's password)
          # User (or group) has to be listed in /etc/sudoers
<sup>8</sup> sudo somecommand # Launch somecommand with root's privileges - can be
                    # restricted for particular commands; /etc/sudoers can
9
                    # contain special settings for particular users/groups
10
u cat /etc/passwd # See all users (including system users)
                                                              ・ 日 マ ふ 雪 マ ふ 印 マ う マ マ マ
                                                                               3
```

Disks and file systems	Types of u	sers Dire	ctory strue	ture	Files and dired	ctories	Permissions	Text	

Directory structure in Linux I

- It is similar also in another UN*X systems
- Directory structure in Linux is similar to macOS (but there it is bit hidden, users usually don't see everything), but very different from Windows "logic"
- Top directory " / " "root"
- Everything else (including disks and network shares) are mounted in subdirectories (/...)
- /bin very basic command line utilities
- /boot bootloader responsible for start of system
- /dev devices representations of disks, CD, RAM, USB devices, ...
- /etc system configuration in plain text files edit them to change system-wide settings (read documentation and comments there)
- /home users' homes

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Disks and file systems	Types of u	sers Dire	ctory strue	ture	Files and dired	ctories	Permissions	Text	

Directory structure in Linux II

- /lib, /lib64 basic system libraries (32 and 64bits)
- /lost+found feature of FS, after crash and recovery of FS, restored files are there
- /media attached disks (USB flash, ...) usually appear there (might be in /var/run/media or /var/media) – subdirectories are automatically created when device is plugged and disappears when unplugged
- /mnt usually manually mounted file systems (but they can be mounted elsewhere according to needs)
- /opt optional, usually locally compiled software
- /proc dynamic information about system processes
- /root root's (admin's) home
- /run temporal ID files (locks) of running processes

Disks and file systems	Types of u	isers Dire	ctory strue	cture	Files and direc	ctories	Permissions	Text	

Directory structure in Linux III

- /sbin basic system utilities
- /selinux SELinux is security framework
- /srv FTP and WWW server data (can be in /var/srv)
- /sys basic system
- /tmp temporary files users have private dynamically created spaces there, used automatically by applications according to need
- /usr binaries (executable applications) and libraries of installed applications
- /var data of most of applications and services, including e.g. database data, system logs, ...
- /windows if on dual boot, Windows disks are commonly mounted here

Disks and file system	s	Types of us	ers Direc	tory struc	ture	Files and direc	tories	Permissions	Text	

Directory structure in Linux IV

- In newest Linux distributions, most of /bin, /etc, /lib, /lib64 and /sbin are mostly in /usr (original locations are just links)
- Can be altered, modified especially on various servers
- E.g. MetaCentrum has storage servers in various locations accessible from frontends and calculation nodes in /storage
- Usually, work only in your home, anywhere else modify files only if you are absolutely sure what you are doing
- Normal user doesn't have permission to modify files outside his directory (with exception of plugged removable media, etc.)
- Try man hier for details



Configuration in /etc (examples)

- Configuration of system services (servers, ...) and behavior
 - Apache web server, database, FTP server, networking, basic system settings, ...
- cron* cron automatically repeatedly scheduled tasks
- **fstab** description of FS mounted during startup
- group list of users and groups
- **passwd** basic settings for users (home directory, default shell, ...)
- resolv.conf DNS settings (part of basic networking)
- shadow users passwords in encrypted form
- **skel** basic directories and configuration for new users
- Much more according to software installed...

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Disks and file systems	;	Types of us	ers Dire	ctory struc	ture	Files and direc	tories	Permissions	Text	

Example of configuration in /etc/ssh/sshd_config

This is the ssh client system-wide configuration file. See
2 # ssh_config(5) for more information. This file provides defaults for
3 # users, and the values can be changed in per-user configuration files
4 # or on the command line.

5 # ...

```
6 Host *
```

7 # If you do not trust your remote host (or its administrator), you 8 # should not forward X11 connections to your local X11-display for 9 # security reasons: Someone stealing the authentification data on the 10 # remote side (the "spoofed" X-server by the remote sshd) can read your 11 # keystrokes as you type, just like any other X11 client could do. 12 # Set this to "no" here for global effect or in your own ~/.ssh/config 13 # file if you want to have the remote X11 authentication data to 14 # expire after twenty minutes after remote login. 15 ForwardX11Trusted yes 16 # ...

Disks and file systems	Types of u	isers Dir	ectory stru	cture	Files and dire	ctories	Permissions	Text	

Everything is (text) file

- In UNIX specifications, everything is (text) file
 - Technically, directory is "just" a file listing its content
 - Text files are easy to read, parse, manipulate
 - Very easily editable (easy to change configuration)
 - Easy to transfer to another system
 - Easily comparable among users/versions/systems
 - UNIX command line tools are the most powerful when processing text files (of any sort, e.g. also genetic data)
- When transferring to and from Windows, be aware of EOL and encoding (slide 76)!
- FAT32 (commonly used for USB flash disks) has limits to maximal file size (~ 4 GB) and range of characters allowed in file name is limited (slide 46), it doesn't support UNIX permissions (breaks executability of scripts)
 - Avoid large single files (or use archives to split large files)
 - In file names keep only alphanumerical characters, dots and underscores (omit spaces and accented characters)
 - Use archives to keep needed permissions (e.g. executability of scripts), see further

Disks and file systems	Types of u	isers Dir	ectory strue	cture	Files and dire	ctories	Permissions	Text	

File names

• Space serves as separator of parameters

Linux allows any character in file name, except slash (/), so including anything on keyboard as well as line break (!) — be conservative...
mkdir My New Directory # Produces THREE directories (mkdir creates dirs; # spaces separate parameters). Solutions:
mkdir "My New Directory" # (you can use single quotes '...' as well) or
mkdir My\ New\ Directory # "\" escapes following character
rmdir My\ New\ Directory # Same problem and solution when removing it
touch * # Creates new empty file named just * (yes, asterisk)
rm * # What would be removed? :-) Solution: rm * or rm '*'

• Files and directories starting by dot (... – . xxx...) are hidden by default (typically user settings and application data in user home)

```
touch .hiddenfile # Let's make empty text file hidden by default
ls # We will not see it (ls lists only "visible" files/directories)
ls -a # We will see it ("-a" to see all - also hidden - files/dirs)
```

Task: Try everything on this slide, also with different file names and characters.

Disks and file systems	Types of users	Directory struct	ure	Files and direct	tories	Permissions	Text	
Types of files								

```
1 ls -la ~
2 -rw-r--r-- 1 vojta users 1685 Feb 25 2019 .bashrc
3 drwxr-xr-x 1 vojta users 1040 Jan 8 09:08 bin
4 lrwxrwxrwx 1 vojta users 28 Jan 11 18:00 .lyxpipe.in -> /tmp/kile-...
5 ...
```

- Regular file ordinary file, marked by dash () on beginning
- Directory in UNIX special type of file, marked by $\frac{d}{d}$ on beginning
- Symbolic link (symlink, "soft link") points to another place, marked by 1, slide 65
- Hard link just another name for existing file, no special symbol, slide 65
- Block and character device in /dev, representations of devices (hard disks, terminals, ...), marked by b or c respectively
- Named pipe pipe can be saved (by mkfifo), looks like a file, more at slide 125
- Socket for communication among processes, also bidirectional, available on network

Disks and file systems	Types of us	sers	Directory stru	ucture	Files and direc	tories	Permissions	Text	

Links

• Symbolic (soft) links (symlinks) – like links on the web – short-cut to another place

• When we delete link, nothing happens, when target, non-working link remains

- 1 ln -s target link_name # Link points to target (existing file/directory)
 2 ls -l bin/cinema5
 3 lrwxrwxrwx 1 vojta users 42 5. dub 2014 cinema5 -> # "1" marks link
 4 /home/vojta/bin/cinema5-0.2.1-beta/cinema5* # "->" points to target
 - Hard links only second name for file already presented on the disk (available only for files): In target link_name
 - If any one of the two files is deleted, the second remains to be fully working

Disks and file systems	Types of us	sers Dire	ectory struc	ture	Files and direc	tories	Permissions	Text	

Owner and group

- Every file has an owner and group for finer setting of rights
- Group can have just one member the user
- System usually shows names of groups and users, but important are IDs (numbers): GID and UID
- Commands chown to change owner requires root privileges
- Commands chgrp to change group often requires root privileges user has to be member of particular group to be able to change ownership to it (if not, root must do it)
- Information about users and groups and their IDs are in /etc/group and /etc/passwd
- Ownership (and permissions, slide 68) are important especially on servers with plenty of users (e.g. on MetaCentrum)
- It is not possible to add particular permissions for particular user on one file/directory there must be special group or ACL must be used (slide 71)

Disks and file systems	Types of u	sers Dir	ectory stru	cture	Files and dire	ctories	Permissions	Text	

Change owner and/or group

1 ls -1 # Shows also owner and group (columns 3 and 4): ² drwxr-xr-x 1 vojta users 80 5. jan 16.12 linuxcourse drwxr-xr-x 1 voita users 1648 31. jan 10.15 presentation 4 -rw-r--r-- 1 vojta users 1944 5. jan 15.18 README 5 drwxr-xr-x 1 vojta users 822 29. jan 10.12 scripts data ⁶ -rwxr-xr-x 1 voita users 1126 5. jan 15.22 web update.sh 7 l # Common alias for 'ls -l' or 'ls -la' (according to distribution) * 11 # Common alias for 'ls -l' or 'ls -la' (according to distribution) o id # Display UID and GIDs of current user ¹⁰ # New owner or group can be defined as name or ID chown newowner:newgroup files # Change owner and group 12 chown -R newowner files # Recursively (with subdirectories) change owner a chgrp -R newgroup files # Recursively (with subdirectories) change group 14 chown --help # Or 'man chown' for more options ¹⁵ chgrp --help # Or 'man chgrp' for more options

• Equally important is to have correct permissions (especially on server) — next slides

Disks and file systems	Types of use	ers Dire	ctory struc	cture	Files and direc	tories	Permissions	Text	

File and directory permissions

• Combination of permissions to read/write/execute for user(owner)/group members/others

Permission	Number	Directory	File
r	4	Read directory content	Read file content
w	2	Write into it (add/remove items)	Write into it, modify, delete it
x	1	Enter it	Launch application (script)

- rwxrw-r-- 3×3 characters for permissions for owner of the file/directory, group it is belonging to, and other users (d on beginning marks directories, 1 links, + ACL, slide 71)
- 764 same as above numbers for each role are summed first one is for owner, second for group and last for others
- Executable scripts and binaries require executable permission (x, e.g. chmod +x or chmod u+x) not supported on FAT drives (USB sticks, memory cards, ...)

Disks and file systems	Types of us	sers Dire	ctory stru	cture	Files and dired	ctories	Permissions	Text	

Permissions examples

1 ls -1 # Shows permissions, links, owner, group, size, date, name $_{2}$ # Only owner can read and write the file; 600: 3 -rw------ 1 voita users 38211 20. jan 09.23 bash history 4 # Owner can write read and write the file, others read; 644: 5 -rw-r--r-- 1 vojta users 2707 29. nov 16.21 .bashrc ⁶ # Owner can enter, read and write directory, others can read and enter it; 7 # 755: ⁸ drwxr-xr-x 41 vojta users 4096 27. pro 09.55 bin 9 # Only owner can read, write and enter the directory, others nothing; 700: ¹⁰ drwx----- 58 vojta users 4096 17. pro 15.45 .config " # Link, everyone can seemingly do everything; 777: 12 lrwxrwxrwx 1 vojta users 37 20. jan 09.33 .lyxpipe.in -> /tmp/kde-vojta/kilemj7d3E/.lyxpipe.in # Check permissions of target! 13 ¹⁴ # Executable (application) - everyone can launch it, but only owner can ¹⁵ # write into the file (change or delete); 755: ¹⁶ -rwxr-xr-x 1 vojta users 2187 27. nov 13.10 strap.sh*

• Permission to "write" also means permission to **delete** it

Disks and file systems	Types of u	isers Dire	ectory stru	cture	Files and direc	ctories	Permissions	Text	

Check and modify permissions

1s -1 # Long list - file names and attributes ² ls -a # All, including hidden files (starting with dot) a ls -F # Add on the end of name "/" for directories and "*" for executable $_{4}$ ls -h # Human readable size units (use with -l or -s) 5 ls --color ## Colored output 6 ls -laFh --color # Combine any parameters you like 7 chmod u/g/o/a+/-r/w/x FILE # For respective user/group/others/all adds # /removes permission to read/write/execute 8 o chmod XYZ FILE # Instead of XYZ use number code of permission 10 chmod -R # Recursive (including subdirectories) u chmod +x script.sh # Make script.sh executable for everyone 12 chmod o-r mydir # Remove read permission from others on mydir 13 chmod 600 FILE1 FILE2 # Make both files R/W only by their owner 14 chmod 000 FILE # No one can do anything - owner or root must add # some permissions before any other action... 15 ¹⁶ chmod 777 * # All permissions for everyone on everything (no recursive) ¹⁷ chmod --help # Or 'man chmod' for more options



Extending permissions – ACL (Access control list) I

- By default, it is not possible to give specific permission to the user who is not owner, nor member of group owning the file
- In ext4 FS it has to be turned on manually (usually it is by default), it is part of Btrfs, XFS and ZFS it is not available on every computer/server
- Command getfacl lists those extra permissions, setfacl sets
- When in use, "basic" tools listing permissions (e.g. 1s -1, ACL in use is marked by + after permissions next slide) sometimes do not show correct result and permissions may work unexpectedly
- Important especially in network environment with many users
- If intensively used, 1s -1 sometimes doesn't show correct permissions (see next slide), it can be confusing and lead into various issues

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Extending permissions – ACL (Access control list) II

- If not in use on a server, relatively high number of groups is required to be able to correctly setup sharing permissions
- MetaCentrum has storages and clusters connected via NFSv4 protocol (see also slide 141) commands getfacl and setfacl do not work there, use nfs4_getfacl, nfs4_setfacl and nfs4_editfacl instead (usage is very similar), see also old MetaCentrum wiki

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• Permissions ("classical" as well as ACL) require some time to practice and master it...

Importance of permissions

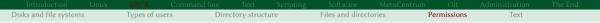
Too permissive (wrong) permissions can lead to data loss, or to data inaccessibility!

Vojtěch Zeisek (https://trapa.cz/)	Linux, command line & MetaCentrum	January 14 to 16, 2025

Disks and file systems	T	ypes of users	Directo	ory structure	2	Files and directo	ories	Permissions	Text	

ACL examples

```
getfacl FILE # get ACL for FILE:
<sup>2</sup> # file: dokumenty
3 # owner: zeisek # Correct
4 # group: zeisek # Correct
s user::rwx # Correct
6 user:nasik:r-x # This is not seen from 'ls -l' output below!
7 group::r-x # This group has only one member, this is fine
8 mask::r-x
• other::--- # Correct
10 ls -1 FILE # Compare this and previous output (This might be wrong!):
u drwxr-x---+ 2 zeisek zeisek 6 17. zář 20.40 dokumenty/
12 setfacl -m u/g:USER/GROUP:r/w/x FILE # Add for USER/GROUP r/w/x right
<sup>13</sup> # E.g. recursively add read permission to user 'arabidopsis data' to
<sup>14</sup> # folder 'dokumenty/arabidopsis' (no extra group is required)
15 setfacl -mR u:arabidopsis data:r dokumentv/arabidopsis
<sup>16</sup> setfacl -R ... # Recursive (including subdirectories)
<sup>17</sup> setfacl -b FILE # Remove all ACL from FILE (combine with -R ...)
```



Set default permissions for new files

- umask sets implicit permissions for newly created files for user
- Syntax is similar to chmod, but reverse (e.g. 027 keeps all rights for owner, for group removes writing and nothing left for others)
 - umask number removes certain permissions
- umask 027 (or other number) is typically set in file \sim /.bashrc
 - means user's home directory
 - . bashrc is user's configuration for BASH (see slide 92)
- Typically used in network environment
- Set with care new permissions will have plenty of consequences different are typically needed for web pages, private files, shared files, ...
- **umask** work recursively for all new files in user home directory it is not possible to set new implicit rules for particular directory

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Disks and file systems	Types of users	Direct	tory struct	ture	Files and direc	tories	Permissions	Text	

Other permissions

- sticky bit new directory/file in shared directory (where everyone can write) will be deletable only by owner (typically in /tmp)
- chmod +t somedirectory

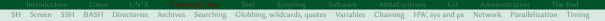
```
2 ls -la /
```

- 3 drwxrwxrwt 22 root root 800 21. jan 18.20 tmp # "t" marks it
 - **setgid** application can have root permission even it was launched by normal user
- chmod u+s someapplication
- 2 ls -al /bin/passwd
- 3 -rwsr-xr-x 1 root shadow 51200 25. zář 08.38 /usr/bin/passwd # Note "s"
 - chattr change of advanced attributes on Linux FS
 - Mostly, there is no need to modify them
- chattr -RVf -+=aAcCdDeijsStTu files
- $_{\rm 2}$ man chattr # See explanation of attributes
- ³ lsattr # List extended attributes

Disks and file systems	Types of use	ers Dire	ctory struc	cture	Files and direc	tories	Permissions	Text	

Text and text - differences among operating systems

- Windows and UNIX have different internal symbol for end of line (new line) EOL
 - UNIX (Linux, macOS, ...): LF $(\setminus n)$
 - Windows/DOS: CR+LF $(\ r n)$
 - Mac v. < 9: CR (\rac{r}) (Mac up to 9 wasn't UN*X, since OS X it is)
- Good text editor (slide 159) can open correctly any EOL, but for example execution of script written in Windows will probably fail on Linux if it has wrong EOL
- Different systems use different encoding
 - UNIX: mainly UTF-8 (Unicode, universal), UTF-16 for Asian languages
 - Windows: win-cp-125X (variants according to region)
 - Older UNIX: ISO-8859-X (variants according to region)
 - Other much less common (historical) types...
 - Important mainly for accented characters
- Text editors can usually open any encoding, but automatic detection commonly fails set it manually, see also slide 160



Command line I

Practical usage of command line tools

④ Command line

BASH and other shells ("command lines")

Screen

SSH - secure shell and screen

BASH

Directories

Archives

Searching

Globbing, wildcards, quotes

Variables

Input, output and their redirecting

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Command line II

Practical usage of command line tools

Information and processes Network Parallelization Timing

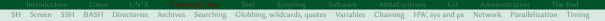
Vojtěch Zeisek (https://trapa.cz/)	Linux, command line & MetaCentrum	January 14 to 16, 2025	78/317

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Launching commands and scripts

- Parameters of commands are separated by space and preceded by one or two dash(es)
- Parameter -h or --help usually gives help for particular command
- Getting help with man command
 - man somecommand
 - Arrows to move up and down, q to quit
 - Type / and then type text to search and hit Enter to search next hit by n
 - Command info more advanced type ? for help
- Parameters can be combined, order doesn't matter (same variants: 1s -1a; 1s -a1; 1s -a1; 1s -1 -a)
- "Long" parameters (--XXX) must stay separated
- Commands (applications) must be in PATH (slide 118) actual directory isn't
 - If the script is is current directory (out of PATH), use ./script.sh or full path
- Custom scripts must have execute permission (chmod +x script.sh)



macOS and Homebrew

- macOS contains outdated versions of many command line utilities with limited functionality comparing to what we are going to use (what is available in modern Linux distributions)
- Several projects provide Linux style way of installation and update of various (not only) command line tools, probably the best is Homebrew
- Xcode must be installed prior installation of Homebrew
- Homebrew contains also plenty of scientific packages, there is also specialized similar source for bioinformatics (and another sciences)
- Tools installed via Homebrew are installed into /usr/local not to interact with system packages
- Derived project is Linuxbrew (works also on Windows subsystem for Linux) useful especially for installation of some special (scientific) software unavailable in main Linux repositories (software resources)

Working with Homebrew

- xcode-select --install # Install compilation tools
- 2 # Install Homebrew
- 3 /bin/bash -c "\$(curl -fsSL https://raw.githubusercontent.com/Homebrew/
 - install/HEAD/install.sh)"
- 5 brew help # Basic help
- 6 # Install updated basic UNIX tools
- 7 brew install coreutils gnu-sed gawk grep bash gcc make wget dos2unix
- 8 brew list # List of installed packages (brew formulae)
- 9 brew info FORMULA # Information about particular formula (package)
- brew search KEYWORD # Search for applications
- n brew update # Update Homebrew
- 12 brew upgrade # Update all packages installed by Homebrew
- 13 brew uninstall FORMULA # Remove Homebrew package (formula)
- 14 brew cleanup # Cleaning after uninstallation
- 15 # Completely remove Homebrew
- 16 /bin/bash -c "\$(curl -fsSL https://raw.githubusercontent.com/Homebrew/
- install/master/uninstall.sh)"

The shell

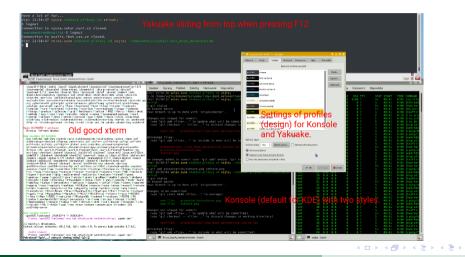
- Many names, many ways how to get it, still the same thing
- Fish friendly interactive shell the command line interface
- Terminal (console)
 - Originally machine used for connection to remote server
 - System uses old fashioned terminal for inner purposes
 - From GUI available using Ctrl+Alt+F1 to F12
 - Changing terminals using Alt+F1 to F12
 - Return back to GUI using Alt+F7
 - Some are used for log outputs etc.
 - Nowadays used "indirectly" with special applications ("emulators")

• Terminal emulator

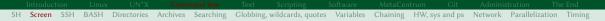
- Application used to get the "terminal" and work in command line
- Every GUI has some Konsole, Yakuake, XTerm, Gnome Terminal, Guake, XFCE Terminal, LxTerminal, ...
- Commonly allow appearance customization font, colors, background, style of notifications, ...
- Launch as many copies as you need (usually allow tabs for easier work) < => < =>

The command line can have various look and feel...

Change colors, font size, etc. for your terminal to like it more and work comfortably



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Screen

Split terminal or keep task running after logging off

- When you log off or network connection is broken during work on remote server, running tasks for particular terminal usually crashes
- Sometimes number of connections to the server is limited
- screen is solution virtual terminals
- Launch screen to start new screen terminal, read some info, confirm by Space key or Enter
- To detach from the screen press Ctrl+A, D (quickly press Ctrl+A, release, press D) screen is still running in background you can even log off
- To return back to running screen use screen -r if only one screen is running, you get back to it
- If more screens are running, use screen -r 1234 (the number is seen from screen -r)
- To cancel running screen press Ctrl+D (or type exit or logout)

Tmux

• More advanced (but not so common) alternative to screen

```
1 tmux # Start new tmux session
2 # Or name the new session (useful if there are more sessions)
3 tmux new -s SomeName
4 # Detach from the session by Ctrl+B, D
5 # List sessions on the server
6 tmux ls
7 # Attach to existing session by name
8 tmux attach-session -t SomeName
9 # Attach to existing session by its number
10 tmux attach-session -t 0
11 # Cancel running session by Ctrl+D or exit
```

- Get help by Ctrl+B, ? (Q to quit)
- Split window by Ctrl+B, % and navigate between them by Ctrl+B, L/R arrow
- It has plenty of options

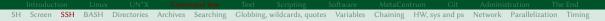
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Login to remote server

SSH - secure shell - encrypted connection

- ssh remoteUser@remote.server.cz
 # When logging first time, check
- $_{3}$ # and confirm fingerprint key
- 4 yes # And press Enter
- 5 # Type remote user's password
- # (nothing is shown when typing)
- 7 # Confirm by Enter
 - Toy server: user names courseu01 - courseu35
- ssh courseuXY@vyuka.natur.cuni.cz
 - If fingerprint key changes, ssh complains a lot possible man in the middle attack
 - From Windows use Putty (see right figure)



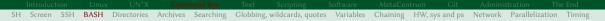


SSH and screen practice

Tasks

- 1 Login via SSH to vyuka.natur.cuni.cz and launch screen.
- 2 Run commands pwd, whoami and 1s -1a. What do they show?
- 3 Detach from screen and logout from the server.
- 4 Login again to the server. Is it same or different process? Why?
- **5** Reattach to the screen same state as before logout from server.
- 6 Open new screen and practice tasks with file names (slide 63).
- ⑦ Detach and re-attach to both screens.
- 8 Close all screen sessions and logout from the server.





BASH and others

- Shell (**sh**) feature rich scripting programming language general specification, several variants
- So called POSIX shell Portable Operating System Interface transferable among hardware platforms (and UNIX systems)
- Interpreter of our commands inserted into command line
- BASH Bourne again shell
 - Probably the most common shell, based on original sh, respecting original specification, adding new features; probably the most common
 - We will use it
- Other variants: **csh** (syntax influenced by C), **ksh** (younger, backward compatible with bash), **zsh** (extended bash; probably the most advanced, not so common), **ash** (mainly in BSD)
 - There are some differences in syntax and features
- Language suitable for easy scripting and system tasks, not for "big" programming, neither for graphical applications

Nice BASH features for easier work (selection) I

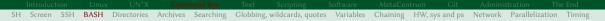
- Arrows up and down list in the history of commands
- List whole history by command history
- Ctrl+R reverse search in history type to search last command(s) containing typed character(s) repeat typing Ctrl+R to search deeper in history
 - When on correct entry, hit Enter or use L/R arrow keys to edit it
 - Ctrl+J exit the search
- TAB list command and files starting by typed characters
- Home / End (or Ctrl+A / Ctrl+E) go to beginning/end of the line
- Ctrl+L clear screen (like clear command)
- Ctrl+Shift+C / V copy/paste the text from terminal emulator
- Ctrl+C cancel running task

Nice BASH features for easier work (selection) II

- Ctrl+D log out (like commands exit or logout)
- Ctrl+U move text before cursor into clipboard
- Ctrl+K move text after cursor into clipboard
- Ctrl+Y paste selection from the above commands
- Ctrl+left/right arrow skip words
- Ctrl+S suspend output of long verbose commands (resume with Ctrl+Q)
- Ctrl+T flip current and left character
- ! xx launch last command starting with xx (use with care)
- Ctrl+X+E start text editor (default, defined in \sim /.bashrc) in current directory
- Can slightly differ (be limited) among various systems, terminal emulators, etc.

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Places to store BASH settings for interactive work in shell

- /etc/bash.bashrc System wide BASH settings can be overridden by user's configuration
- ~/.bashrc File is loaded each time user creates new session (typically opens new terminal window)
- ~/.bash_profile Used specifically (not in every system) when user is using remote connection (e.g. SSH) user can have different settings for local and remote work
- **/etc/profile** System wide profile file can be overridden by user's configuration
- ~/.profile Settings loaded when user logs-in (mainly for language settings), sometimes used by remote connections
- Note: BASH scripts are non-interactive shells they do not read settings above there are no aliases etc., but they inherit some settings (PATH, language, ...) and they can read global (not local) variables

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BASH settings (popular examples)

Write them into BASH configuration file

- In any text editor open \sim /.bashrc (and/or \sim /.bash_profile) and edit it
- Behavior of BASH can be set to fit user's needs
- Terminal emulators allow to set custom fonts and colors, ...
- Prompt can be colored using custom values of PS1 and PS2 variables (export PS1='...'), see examples and search

```
eval "$(dircolors -b)" # More colors for outputs (typically 1s)
```

- ² # Colored GCC warnings and errors (useful for compilation)
- 3 export GCC_COLORS='error=01;31:warning=01;35:note=01;36:caret=01;32:
 - locus=01:quote=01'
- 5 # Example of more colorful prompt (do the same for PS2)
- 6 export PS1='\[\033[0;34m\]\u\[\033[0m\]@\[\033[0;32m\]\h\[\033[0m\]:

Examples of BASH settings

- $_{\rm I}$ # Set custom default editor (Ctrl+X+E and other cases)
- 2 export EDITOR='nano'
- 3 # Ignore repeated entries in bash history (stored in ~/.bash_history)
 4 HISTCONTROL='ignoreboth'
- 5 # Maximal length (number of lines) of bash history (~/.bash_history)
 6 HISTFILESIZE='100000'
- 7 # Following two settings save history from multiple terminals
- 8 # Normally, only history from last time opened terminal is kept
- 9 shopt -s histappend # Append to history, don't overwrite it
- ${\scriptstyle \scriptstyle 10}$ # Save and reload the history after each command finishes
- n export PROMPT_COMMAND="history -a; history -c; history -r;
- 12 \${PROMPT_COMMAND}" # Note its recursive behavior
 - shopt can set various shell options, see e.g. https: //www.geeksforgeeks.org/shell-scripting-shopt-command/ (it can be used also in script to set some specific shell behavior)

Aliases and BASH settings I

Alias is short cut – instead of very long command write short alias

¹ # Define new alias ² alias ll="ls -l"

- Can be stored in ~/.bashrc (or ~/.profile or ~/.bash_profile)
- If there are plenty of them, aliases can go to ~/.alias and ~/.bashrc then contains test -s ~/.alias && . ~/.alias || true

```
# After adding new aliases to ~/.bashrc or ~/.alias or so reload it
source ~/.bashrc # Reload BASH settings to load newly aliases
# Popular ls aliases
alias ls="ls --color=auto" # Make output of ls colored
alias l="ls -laF" # Long list (add details) with hidden files
alias ll='ls -l' # Long list (add details) without hidden files
alias lh='ls -lha' # Long list (add details) with human readable sizes
```

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Aliases and BASH settings II

```
alias md='mkdir -p' # Making directories
```

```
2 alias rd='rmdir' # Removing directories
```

```
3 alias o='less' # Text file viewer
```

```
4 alias grep='grep --color=auto' # Enable color in grep
```

```
<sup>5</sup> alias df='df -h' # Always human readable output of df (disk free)
```

```
6 # Easier history listing
```

```
7 alias his="history | grep" # Use e.g. 'his ls' to list last 'ls' usage
8 # Add aliases pointing to software installed outside PATH, ...
```

```
9 # Add ~/.local/bin to PATH (directories with commands and scripts)
10 export PATH="${PATH}":~/.local/bin:~/bin
```

- ~/.bashrc can contain anything (technically it's just BASH script), functions, whatever needed
- ~/.bashrc commonly contain definitions of variables
- Other shells than BASH (KSH, ZSH, ...) have their own configuration files

Directories

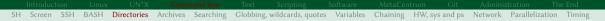
- When using cd, cp, mv, ... use <TAB><TAB> key suggesting matching names of files and directories and save repeated and unneeded typing
- In command line, **user is always in some directory** it's crucial to train fluent moving among directories and manipulation with files
 - If lost among directories, run **pwd** to find out current directory and **1s** to see what is around
- pwd # Print working directory where we are right now
- 2 cd # Change directory (just "cd" or "cd ~" goes to home directory)
- 3 cd .. # One directory up; cd ../..; cd ../../another/directory/
- 4 cd relative/path/from/current/position # Go to selected directory
- 5 cd /absolute/path/from/root # Absolute path starts by "/"
- 6 cd # Go to previous directory
- 7 tree # Tree like hierarchy of files and directories
- 8 tree -d # List only directories; see tree --help
- 9 tree -L 2 # Only up to second level; combine: tree -d -L 3

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Directories and files

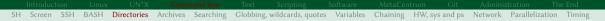
du -sh # Disk usage by current directory, -s for sum, -h for nice units ² mkdir NewDirectory # Make directory ³ rmdir DirectoryToRemove # Remove empty directory 4 ls # List directory content # Try parameters -1, -a, -1, -F, -h (with -1 or -s), --help6 rm -r # Recursive delete - remove also non-empty directories 7 my from to # Move files/directories (also for renaming) 8 mv docs to/sub/directory/ # Move 'docs' to 'to/sub/directory/' g cp from to # Copy, -r (recursive, including subdirectories) # -a (keeps all attributes), -v (verbose) 10 " # Copy 'XXX' (recursively with subdirectories and everything) in the ¹² # upper directory into 'sub/directory/' 13 cp -a ../XXX sub/directory/ 14 # Copy 'doc.txt' from home directory into current directory ¹⁵ cp ~/doc.txt . # Dot stands for current directory ¹⁶ file somefile # Information about questioned file (what it is, ...) 17 xdg-open somefile # Open file by graphical application as in GUI



Tasks on the remote server I

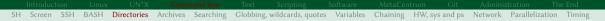
Login via SSH to vyuka.natur.cuni.cz.

- ② Get your path by pwd.
- **3** Go to /srv/scripts_data (with cd) and explore its content (1s).
- Ist permissions in /srv/scripts_data (slide 68). What do they show? What can you do with the content?
- 6 How much space does /srv/scripts_data consume?
- 6 Go back to home directory (by cd).
- ⑦ Create new directory in your home directory (mkdir).
- 8 Copy content of /srv/scripts_data into your newly created directory (cp).



Tasks on the remote server II

- Sename that directory with scripts and data using mv to any custom name. Who is owner of the files in origin location and in new location? Why?
- ① Explore your home directory and its content by command ls and tree and some files by command file. Which hidden files and directories are there? What could it be?
- Change permissions of the files so that only you can read, write and execute them (chmod).
- ⑦ Create other directory, see it and then remove (rmdir).
- B Can you access directories of another users? Why? If yes, what are your permissions there? Explain it.
- What are some permissions in /? Why?
- Define some alias (by running alias command, or edit ~/.bashrc and reload it) and use them.



Tasks on the remote server III

- Create directory in your home directory and share it with another user so she/he can write there anything (using e.g. touch somefile or mkdir somedirectory) (work e.g. in pairs). Use everywhere as restricted permissions as possible. Can you figure out solution with or without ACL (slide 71)?
- Practice moving between /srv/scripts_data and your home directory. Use cd and TAB.
- **1** Within /srv/scripts_data list by single command only jpg and txt files.
- Oreate in your home directory new directory scripts and copy there with single command all shell scripts (*.sh) files from /srv/scripts_data
- ② Copy anywhere into your home /srv/scripts_data and by single command remove all jpg and sh files there.

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Midnight Commander

- mc to launch MC (F10 to quit), can be used with mouse
- Move (F6), copy (F5), delete (F8), files/directories, TAB to switch panes
- Connect to SSH/(S)FTP, ...
- Edit (F4) or view (F3) text files
- F2 for quick menu
- F9 for top menu
- And much more...
- Impossible to live without it :-)
- Task: Which of the previous tasks can you solve with it? Try it.

Left File	Contand Options	Eight		re/dokumenty		
	User menu Birectory tree		tine 10:12	in Kao		Size Hodify time
Conditation	Find file	8-7	2014	(bat anak		40% 17.0rc 09:3
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-Skype			21:01	/jazyky		4095 4.5ep 09:4
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.natlab		4056 117.5ep	201.1			
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Vojtěch Zeisek

Linux, command line & MetaCentrum

Compressing and decompressing archives

- gzip, bzip2, xz and lzma are able to pack only one file use them together with tar to pack multiple files (when used without tar they move file into archive)
- In Linux, gzip (and less bzip2) are the most commonly used
- Rar and arj are not used at Linux/UNIX at all
- Zip is probably the most portable between Linux/UNIX and Windows
- 1zma and xz have excellent compression, but can be very slow, use similar algorithm, often confused



https://xkcd.com/1168/

to 16, 2025

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Vojtěch Zeisek (https://trapa.cz/)	Linux, command line & MetaCentrum	January 14

Compressing and decompressing archives

Archive *.tar *.tar.gz / *.tgz *.tar.bz / *.tbz / *.tar.bz2 *.tar.xz *.tar.lzma *.gz Compressing command

tar cvf archive.tar file1 file2 file3 tar czvf archive.tar.gz/.tgz file1 file2 tar cjvf archive.tar.bz/.tbz/.tar.bz2 file1 file2 file3 file4 tar cvJf archive.tar.xz file1 file2 file3 tar cvf - file1 file2 file3 file4 | lzma > archive.tar.lzma gzip file

bzip2 file xz -zv file Izma file

zip -r archive.zip file1 file2 file3 file4

Decompressing command tar xvf archive.tar tar xzvf archive.tar.gz/.tgz tar xivf archive.tar.bz/.tbz/.tar.bz2 tar xvlf archive.tar.xz lzcat archive.tar.lzma | tar xvf gunzip archive.gz bunzip2 archive.bz2 xz -d archive.xz unlzma archive.lzma

unzip archive.zip

* bz2

*.xz

*.lzma

*.zip

(日)

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Tasks with archives

• Compress (and decompress) text file Oxalis_HybSeq_nrDNA_selection_

alignment.fasta from scripts_data with various compressing tools.

- 2 Compare sizes of original file and compressed outputs.
- G Compress (and decompress) all foto_oxalis_*.jpg (Oxalis photos) together from scripts_data with various compressing tools.
- ④ Compare sizes of original files and compressed outputs.
- Which compression tool seems to be the best? In terms of compressing ratio and time needed for compression.
- **6** Is more effective compression of text files or images? Why?
- Why is even plain tar (without compression, it requires gzip, bzip2, xz or lzma to add compression) useful with FAT disks (it applies also for another tools)?
- 8 Search the Internet to find out how to unpack arj and rar archives from command line.

Vojtěch Zeisek

Find – looking for files

find <where> <what> <what to do> # The most powerful searching tool: find /... -type d/f -name XXX -print # Most common usage

- First **find**'s parameter is location to search absolute or relative, "___" means current directory (the only compulsory parameter)
- -type for only directories d or only files f (without this parameter, files as well as directories are looked for)
- -name of the searched files/directories supports wildcards (*, ? and [...]), see globing (slide 110)
- -print is default action prints list of results
- -exec runs some command with results (some operation, not just listing)
 - All following arguments are argument of the command until "; " is encountered
 - '{}' is replaced by the current file name being processed
 - Those constructs might require protection by escape ("∖") or quotes not to be expanded by
 shell

Vojtěch Zeisek

Linux, command line & MetaCentrum

January 14 to 16, 2025

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Find examples I

Apply some (or something similar) of them to the toy data

Find in /home/\$USER/ all JPG files containing string "oxalis" ² find /home/\$USER/ -name "*oxalis*.jpg" -print ³ # Find in scripts data all JPG files and resize them to 1000x1000 px 4 find scripts_data -name "*.jpg" -exec mogrify -resize 1000x1000 '{}' \; 5 # Another possibility with xargs (it chains commands - reads input from ⁶ # stdin and execute command with given arguments, using all CPU threads) 7 # Note in the example below -print is not needed as it is default action 8 find photos/ -name "*.jpg" | xargs mogrify -resize 1000x1000 9 # How many directories are there in the books directory 10 find books/ -type d -print | wc -1 # wc -1 calculates lines " # Change permissions of all files within "files" directory to 640 find files / -type f -exec chmod $640 ' \{\}' \}$; ¹³ # Find all R scripts in ~/Documents and find in them lines with "DNA" 14 find ~/Documents -name "*.r" -print | xargs grep -nH DNA # Or $_{15}$ find ~/Documents -name "*.r" -exec grep -nH DNA '{}' \;

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Find examples II

Apply some (or something similar) of them to the toy data

- **find** is extremely versatile and useful tool master it (see also **man find** for help)
- -print is default action if it is missing and there is no other actions, results are printed to the screen
- # Find all executable files within current directory and list them ² find . -executable -type f -print ³ # Delete empty directories within 'doc' directory 4 find doc/ -type d -empty -execdir rmdir '{}' \; 5 # Copy all *.sh files from /home to ~/scripts 6 find /home -name "*.sh" -exec cp '{}' ~/scripts/ \; 7 # Search for file long text.txt (exact name) in your home directory 8 find ~ -name long text.txt -type f -print 9 # Find in current directory files from 1 to 100 MB 10 find . -type f -size +1M -size -100M " # Search in home dir for files named "*.jpg" or "*.txt" and print them ¹² find ~ -name "*.jpg" -o -name "*.txt" # '-print' is default, can be omitted

Looking for applications and files

updatedb # Must be regularly launched to get "locate" to work # It is usually regularly launched by cron task (see further) a locate somename # Searches for files/directories in "locate" database apropos keyword # Searches for command descriptions containing keyword ⁵ which app # Full path to application (shell command) ⁶ where is app # Path to source code, executable and man pages for the command 7 # Test if executable command exists (good for scripts) 8 # If "Application" is missing, script ends with error o command -v Application >/dev/null 2>&1 || { echo >&2 "Application is required but not installed. Aborting."; exit 1; } 10 u type Application >/dev/null 2>&1 || { echo >&2 "Application is required but not installed. Aborting.": exit 1: } 12 ¹³ # More reliable than 'which Application || { echo XXX; exit 1; }' exit 1 # "exit" use to be added (with various numbers) after any error # to send term signal 1 - for better handling of various errors. 15 # Every termination has exit status number - 0 is normal exit. 16 # Exit status 1 and higher number is various error. 17

Searching tasks

- Use locate to find file long_text.txt on the server. Is the output absolutely correct? If not, why?
- 2 Where is executable of mc? Why can be such information useful?
- Which software is related to keywords permission and compress (use e.g. apropos)? Use man to explore some of them.

Tasks with find

- Find all *.vcf.gz files in whole /home. Why do you get errors for some directories?
- 2 Compress, see and decompress all shell scripts in your home directory.
- Change permissions of all content of your home directory so that no one else can access it.
 Consider hidden files, directories and scripts.
- 4 List all directories in /etc up to second level.

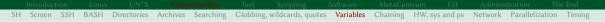
BASH globing and wildcards

- BASH itself doesn't recognize regular expressions (from slide 191) its wildcards have some of functions of regular expressions and can look similarly, but behave differently — Do not confuse!
- ? Replaces any single character
- ***** Replaces any number of any characters ($1s a^*$ lists all files starting with "a")
- [] Range or a list [abcdef] and [a-f] are same
- [!...] Reverse previous case (!) any character except those listed
- {} Expansion (terms inside are separated by commas ,) all possible combinations (see next slide for examples)
- \ Escapes following character and it doesn't have its special meaning (e.g. * means literally asterisk * and not "any number of any characters" as usually)
- For details see man 7 glob and man 7 regex
- Useful e.g. to list only subset of files or to provide file selection as input for some command $_{\odot}$

Brace expansion and quotes

echo a{p,c,d,b}e # ape ace ade abe - all combinations
echo {a,b,c}{d,e,f} # ad ae af bd be bf cd ce cf - all combinations
3 ls *.{jpg,jpeg,png} # Expansion to *.jpg *.jpeg *.png, same as:
4 ls *.jpg *.jpeg *.png
be certified atta (* D[12] foota ba2 # Come as * D1 foota ba2 * D2 food

- 5 ls scripts_data/*_R[12].fastq.bz2 # Same as *_R1.fastq.bz2 *_R2.fastq.bz2
 - Text in single quotes ('...') preserves the literal value of each character within the quotes
 - Text in double quotes ("...") preserves the literal value of all characters within the quotes except of dollar (\$), back tick (`) and back slash (\) handling variables
 - A double quote may be quoted within double quotes by preceding it with a backslash (\\" means literally "double quote")
 - Text between back ticks (`...`) or within \$(...) will be evaluated and then used as command or argument (see next slide for examples)
 - Syntax with back ticks is deprecated, keep using **\$(...)** instead
 - This is important when handling file names with non-Latin characters, when working with variables (from slide 113), printing various information within scripts (e.g. slide 121), etc.



Variables in BASH

- Variables contain various information (where to look for the executable programs, name of the computer, various settings, input files, ...)
- Can be local (within a script for some temporal purpose) or global available for all processes (and users)
- Names commonly written in CAPITALS (just a costume)
- Popular and useful variables
 - **HOME** location of user's home directory
 - **HOSTNAME** network name of the computer
 - LANG language settings, encoding, similarly variables LC_*
 - **PATH** paths where to look for applications all applications have to be in **PATH** or called directly (slide 118)
 - SHELL shell in use (bash or something else)
 - USER user name
 - And many more, commonly specific for particular server

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Work with variables

- Names start with \$, e.g. \$HOME, but declaration is without \$, e.g. MYVAR='XXX'
- Variable defined within shell session, script, function, etc. will disappear as soon as the session, script, function, etc. is terminated it must be exported, defined in ~/.bashrc or so to be preserved
- printenv # Get all environmental variables and their values ² export -p # Get all exported variables and their values ³ declare -p # Get all declared variables and their values 4 echo "\${VARIABLENAME}" # Get value of particular variable s echo "\${PATH}" # Get path where to look for applications ⁶ VARIABLE='variablevalue' # Set new variable and its value # Or replace existing variable by new value 8 export EDITOR='/usr/bin/vim' # Set new default text editor LISTFILES="\$(ls)" # Get output of command 'ls -1' into the variable echo "\${LISTFILES}" # See content of the variable LISTFILES export GREP OPTIONS='--color=auto' # Colored grep (see further) ¹² unset VARIABLENAME # Drop variable and its value

How quotes influence reading of variable content I

• As soon as variable value (content) should contain anything else than plain Latin characters and numbers, or should combine with another variable, be careful...

```
A=abcdef # Set new variable (no special characters allowed)
<sup>2</sup> echo $A # See variable's content
abcdef # It works
4 echo '$A' # Single guotes preserve literal value
5 $A # We see variable's name, not its content
_{6} echo "$A" # Double quotes preserve literal value, except $, `, \
7 abcdef # This also works; not needed here
8 echo `$A` # Text between back ticks is evaluated as a command and launched
abcdef: command not found # There is no command "abcdef"...
<sup>10</sup> echo $($A) # Same as `...`, this is now recommended way, `...` is legacy
              # Commonly used to fill variable by output of some command, e.g.
1.1
             FOTOPROCESS=$(find "${DATADIR}" -type f -name "*.f*q")
12
<sup>13</sup> echo "Hi, dear $USER" # Compare this and following command...
<sup>14</sup> echo 'Hi, dear $USER' # Single quotes do not evaluate variables
                                                             (ロ) (型) (ヨ) (ヨ) (ヨ) (マ)
```

How quotes influence reading of variable content II

- B=abcd\$e # The content will be "abcde + \$e" or "abcd" (if \$e is missing)
- ² echo \$B # abcd
- 3 C=abcd\\$e # \ escapes next character it is loosing its special meaning
 4 echo \$C # abcd\$e
- ₅ C='abcd\$e' # '...' keep literal value of the content; as above
- 6 # Next command breaks shell incomplete quotes " pres then Ctrl+C
- 7 D=ab"cde # The variable should contain incomplete quotes ", it fails 8 echo \$D # Nothing - empty
- 9 E=ab\"cde # \ escapes next character it is loosing its special meaning 10 echo \$E # ab"cde
- $_{11}$ E='ab"cde' # '...' keep literal value of the content; as above
- 12 F=abc\${USER}de # \$USER wouldn't work {} are needed
- 13 echo \$F # abcvojtade # To add output of command into the variable
- 14 G="abc\$(echo \${USER} | tr [:lower:] [:upper:])de" # Modification of var.
- $_{15}$ echo $G \ \ \ See$ what happened with content of USER
- 16 H=abc def # Error: command "def" not found... Why? Fixing:
- 17 H='abc def' # "echo \$H" outputs "abc def" typical problem with paths

How quotes influence reading of variable content III

- As soon as variable contains only Latin alphanumerical characters, assignment like MYVAR=whatever works, but it is not recommended
- If variable should contain another variable, special characters, etc, use double quotes, e.g. WORKDIR="/home/\$USER/data"
 - It might be called like echo \$MYVAR, but if there would be non-standard characters anywhere, it'd fail, so prefer "\$MYVAR" (it might work without quotes, but don't risk it) or "\${MYVAR}" as the most reliable way
- If variable should contain any special character (including space), or you wish to be sure you keep it's literal value, use single quotes, e.g.
 MYDATA= '~/My Doc/exp 1/data.fsa' (and then "\${MYDATA}")
- Similar for using variables
 - Using **\$MYVAR** is fine if it doesn't contain anything special (but are you really sure?)

Manipulating with content of variable

- It is possible to change/remove extension (suffix) of variable, do simple search and replace with its content, etc. (useful in scripts e.g. for input and output files)
- Search and replace syntax is related to sed (slide 175)

```
MYVAR='oxalis_assembly_6235.aln.fasta' # Assign new variable
2 echo "${MYVAR}" # See it - it works: oxalis_assembly_6235.aln.fasta
# Remove the '.fasta' extension
4 echo "${MYVAR%.fasta}" # oxalis assembly 6235.aln
5 # Replace extension '.fasta' with '.fsa'
6 echo "${MYVAR%.fasta}".fsa # oxalis assembly 6235.aln.fsa
7 # Remove any last extension
8 echo "${MYVAR%.*}" # oxalis_assembly_6235.aln
• # Replace 'aln' within variable name with 'aligned'
ro echo "${MYVAR/aln/aligned}" # oxalis assembly 6235.aligned.fasta
" # More complex manipulations with variable content (try to avoid this)
12 echo "$(echo "${MYVAR}" | sed "s/assembly/${USER}/")"
# sed allows usage of variables (sed "s/pattern/$SOMEVAR/", see further)
```

The PATH variable

- Lists directories (separated by colon :) where the current shell searches for commands
- If some software is installed outside standard locations, the user must specify the full path (or update the **\$PATH**)
- In case there are two commands with the same name (e.g. /usr/bin/somecommand and /home/\$USER/bin/somecommand), the order of directories in \$PATH matters the first occurrence is used, any possible later ignored
- Computing clusters (like MetaCentrum) use to have special command (e.g. module) to load particular software (including particular version) by extending user's **\$PATH**
- echo \$PATH # See the \$PATH variable. Sample output is on the next line:
- 2 /home/\$USER/bin:/usr/local/bin:/usr/bin:/opt/bin:/sbin:/usr/sbin
- # Adding new directory to \$PATH
- 4 export PATH="\${PATH}":/some/new/directory # Ensure to add original \$PATH
- # Do not overwrite \$PATH there would be only the new directory
- 6 export PATH=/some/new/directory # Wrong! Old \$PATH is missing!

Reading variables from command line and as output of other commands

This is especially useful in scripting to read input from users or from another commands

```
# Reading variable from user's input from command line
<sup>2</sup> # (some interactive script interacting with the user)
3 read X # We will read new variable from input (do not use "$" here)
<sup>4</sup> 10 # Type any value and press Enter
5 echo $X # Get value of the variable
6 10 # It works
_7 echo "$((1 + $X))" # Sum of 1 and variable $X
8 # Output some command into variable
<sub>9</sub> Y=$(command) # Set as variable output of command
10 echo $Y # Y will contain output of command
" # "command" from previous lines can be e.g.
12 cat somefile.txt # Read content of somefile.txt; or
13 find . -name "*.txt" # Save list of matching files
14 WORKDIR="$(pwd)" # Save current directory into variable
15 ls -1 | head -n 1 # First file/directory in the current directory
<sup>16</sup> unset X # Destroy this variable
```

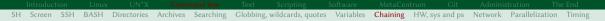
BASH expressions

Basic arithmetic operations and more with BASH

```
echo ((5 < 7)) # Is 5 smaller than 7? TRUE (1)
_2 echo ((3 > 4)) \# Is 3 greater than 4? FALSE (0)
g echo $((16 / 3)) # Division (without decimal part)
4 echo $((16 % 3)) # What remains after aritmetic division
_{5} x = ((1 + 6)) \# Result will be in 'x' - save output into variable x
6 echo $x # See content of $x
_{7} x=1 # Set x to 1
o echo $v # See result
v = ((x + 1)) \# Will this work? Why?
n echo $v # Result
<sup>12</sup> echo $(expr length "MetaCentrum and Linux") # Get length of chain
<sup>13</sup> # String of 5 characters starting at position 10 of the text
echo $(expr substr "MetaCentrum and Linux" 10 5)
15 # Does 1st chain contain 2nd chain (how long)? Get position of first hit
<sup>16</sup> echo $(expr index "GNU Linux" "Linux") # If no overlap, return value is 0
```

Notes about variables, expressions and quotes and more

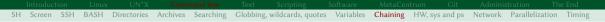
- expr works with various operands (see man expr) it used to be utilised also for simple computations, \$((...)) is now preferred
- Exported variables will be lost when logging off
- To make variables permanent, add export commands into ~/.profile or ~/.bash_profile, or ~/.bashrc (according to shell and its settings)
- "<mark>~</mark>" means home directory
- \$ marks variables
- N escapes following character it will not have its special meaning (space to separate arguments, ... next slide)
- If variable is going to contain any special character (?, ., *, ...), the value must be quoted "..." allow escaping of special character or inclusion of another variables, '...' keeps absolutely literal value



Chaining commands I

- Key feature of BASH work with individual commands as with Lego to get new functionality
- & command will be launched in background, terminal is available for next typing: firefox & (when launching graphical application, hit Enter afterward if there is no active command line prompt)
 - If the application has any output, it goes to the screen, so it can be bit messy...
- && second command is launched only when first command exits without error (exits with status 0): mkdir NewDir && cd NewDir
- ; second command is launched regardless exit status of the first one: kshfskcbd; hostname
- {...} commands within curl brackets are launched as one block
 - Closing bracket } must be either on new line or preceded by semicolon (... ; })

A = A = A = A



Chaining commands II

- || second command is launched when first command fails (has non-zero exit status):
 - cd newdir || { mkdir newdir && cd newdir; }
 - Easy way how to do something when previous command fails, either exit script

(... | | exit 1) or somehow fix it (see above), report problem

(... || {echo "It failed!" && exit 1; }) or so

 | - pipe - redirects standard output of one command into standard input of second command: compare mount and mount | column -t

- Chains commands, basic redirecting method common e.g. for various data parsing
- One of key features for commands and scripts processing scientific data, e.g.
 bwa mem ... | samtools view -bu | samtools sort -o sample.bam
- Behavior in shells other than bash might be little bit different

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Standard input and output and redirects

- Standard input (stdin) is standard place where software takes input (keyboard and terminal) and writes results to standard output (stdout) – typically monitor (or file)
- Standard error output (stderr) is target of error messages typically also monitor (but can be log file or so)
- > redirects output into new place (file, device, another command, ...)

• >> adds output to the end of the file (> rewrites target file)

grep root /etc/group >> users # Add new information into existing file cat users # See result

• Task: Practice chaining and redirects from previous and this slide. What is it good for?

Redirects of input/output

/dev/null – "black hole" – can discard anything

command 2> /dev/null # Discard only errors (note "2" for errors only)
command > /dev/null # Discard all output (no logging or onscreen output)

- /dev/stdin standard input (typically keyboard)
 - In case application reads files, not from standard input:

echo "Žlutoučký kůň úpěl ďábelské ó" | iconv -f utf-8 -t cp1250 /dev/stdin

- /dev/stdout standard output
 - Typically screen, commonly redirected into file
 - We wish to see errors which would be discarded otherwise:

command 2> /dev/stdout # Errors go to screen (typically), not to log

- /dev/stderr standard error output
 - Typically screen or log file, right place to send errors to:
- echo "error" > /dev/stderr
- 2 command 2> /dev/stderr # Errors go to standard error log

Redirects of standard input and output I

Common way how to save output of some command(s)

If file directory_listing.txt exists, will be overwritten
ls -la > directory_listing.txt
cat directory_listing.txt # See result (same as running "ls -la")
If file directory_listing.txt exists, new content will be appended
ls -la >> directory_listing.txt # See result 'cat directory_listing.txt'
We are outputting 'ls -lh' to 'awk' and not to screen, printing only
selected columns, and parsing with 'column -t' for tabular display
ls -lh # Compare outputs of the 3 commands starting with 'ls -lh'
ls -lh | awk '{ print \$NF, " ", \$5}' # See further more info about AWK
ls -lh | awk '{ print \$NF, " ", \$5}' | column -t

Tasks with redirects of standard input/output

1 Try everything on this and following slide, be sure to understand the redirects.

2 Try to figure out some other example regarding your practical needs.

Redirects of standard input and output II

- # Add error output to the end of standard output file 2 # Note: In the examples below command "commandX" does not exist -³ # it produces error "command not found" to be recorded by the log 4 # and because of redirect, the error is not shown in the terminal. ₅ command > outputfile.log 2>&1 # Example: 6 { commandX; ls; } > outputfile.log 2>&1 7 cat outputfile # See result 8 # Compare with following. What is the difference? $_{9}$ { commandX; ls; } > outputfile.log # Where does error and output go? ¹⁰ # Compare two following commands. What is the difference? 1 { commandX: ls; } > outputfile.log 2>&1 # Inspect outputfile.log 12 { commandX: ls; } >> outputfile.log 2>&1 # Inspect outputfile.log ¹³ # Add error output to the error log text file 14 command >> outputfile.log 2> error.log # Example: 15 { commandX; ls; } >> outputfile.txt 2> error.log 16 cat outputfile.txt # See results
- 17 cat error.log # See results

Examples of redirects and pipes when working with molecular data I

Extract and sort depth of coverage (how many times was each position ² # sequenced) in genomic VCF with multiple individuals 3 zcat arabidopsis.vcf.gz | grep -o "DP=[0-9]\+" | sed 's/^DP=//' sort less 4 # Convert DNA sequence from FASTQ to FASTA (two of many options) 5 # Discard FASTO quality scores and keep only the sequence and its name 6 bzcat Oxalis_hirta_R1.fastq.bz2 | sed -n '1~4s/^@/>/p;2~4p' > \ Oxalis hirta R1.fasta 8 bzcat Oxalis hirta R2.fastq.bz2 awk $' \{ if(NR\%4==1) \}$ {printf(">s\n",substr((0,2));} else if(NR%4==2) print;}' > \ 0 Oxalis hirta R2.fasta 10 # See both sequences in one view 12 less Oxalis_hirta_R{1,2}.fasta ¹³ # Mapping of trimmed Illumina FASTO reads to reference FASTA sequence 14 # and creation of BAM containing the alignment (reference and mapped ¹⁵ # reads, one BAM for each sample) 16 bwa mem reference.fasta input R1.fastg input R2.fastg | samtools view \ -bu | samtools sort -1 9 -o mapped.bam 17

Examples of redirects and pipes when working with molecular data II

```
# How many FASTO reads are there in the file
2 echo "$(("$(wc -1 file.fastq)" / 4))"
# Count number of *.FNA or *.fasta files in current directory
4 find . -maxdepth 1 -name "*.FNA" -o -name "*.fasta" | wc -1
5 # Same as above, saving output to the file
_{6} echo -e "Hey, {USER}, Number of FASTA files: t (find . -maxdepth 1 \setminus
    -name "*.FNA" -o -name "*.fasta" | wc -1)"
8 # Compressing all *.fq or *.fastq files in parallel using all CPU threads
9 find . -name "*.f*q" -print | parallel bzip2 -v9 '{}'
<sup>10</sup> # Statistics using BCFtools for all *.vcf.gz files in current directory
n echo "Statistics of SNPs in VCF files using bcftools"
<sup>12</sup> for VCFGZ in *.vcf.gz; do
    echo "Processing ${VCFGZ} at $(date)"
13
    bcftools stats --threads 2 -F reference.fasta "{VCFGZ}" > \
14
      ${VCFGZ%.vcf.gz}.stats.txt || exit 1
15
   echo
16
done
```

Which system are we using?

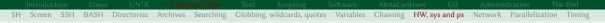
- uname -a # Information about Linux kernel (version, ...)
- ² lsb_release -a # Information about Linux distribution release
- 3 cat /etc/os-release # Similar to above command
- 4 lscpu # Information about CPU; better than 'cat /proc/cpuinfo'
- 5 lsusb # List of devices on USB
- 6 lspci # List of PCI devices (graphic card, network card, ...)
- 7 lspci | grep -i vga # Get information about graphical card
- 8 lshw # Complete list of hardware; e.g. 'lshw -C memory' for RAM
- 9 hwinfo # Complete list of hardware; "hwinfo --network" for network devices 10 neofetch # System information tool
- n free -h # Available memory (RAM) and swap, -h for nice units
- 12 df -h # Free space on disk partitions, -h for nice units
- 13 1smod # List loaded kernel modules
- $_{14}$ uptime # How long is the system running, number of users, average load
- $_{\scriptscriptstyle 15}$ date # Date and time plenty of options for formatting
- 16 mount # Information about mounted file systems
- 17 findmnt # Display mounted devices in tree structure

Processes – every running program has its own process ID

top # Listing of processes, quit using "q" ² htop # Nice listing of processes (better version of top), quit using "q" # Allows also termination of processes etc. 4 pstree # See running processes with child processes, recursively ⁵ ps # processes related to actual terminal 6 ps ux # All user's processes 7 ps aux # All processes 8 pgrep application # Return PID (process ID) of application 9 # kill (terminate) process by name or process ID (PID) ¹⁰ # Find which PID has application to terminate pgrep geany 12 14639 # Process ID (PID) of respective process ¹³ # Kill (stop by SIGTERM) selected application according to above PID 14 kill -SIGTERM 14639 # SIGTERM is "nice" termination, SIGKILL "brutal" 15 kill -SIGTERM \$(pgrep geany) # Two above commands in one step; note \$() 16 killall -SIGTERM geany # Select by name (more processes with same name)

Processes and users

nice - how much resources will task use: from -20 (high priority - not ² # "nice" process) to +19 (low priority - very "nice" process), default 0 a nice -n 7 hard task.sh # set priority 7 for newly launched task renice 15 16302 # Change priority of PID 16302 to 15 ⁵ sudo renice 15 16302 -u USER # Change priority of USER's process 6 whoami # What is my user name 7 id # Information about current user (user ID and group IDs) ⁸ who # Who is logged in ₉ w # Who is logged in, more information ¹⁰ users # Plain list of currently logged users finger # Information about users on current terminals 12 last # Last logged-in users 13 passwd # Change password 14 passwd USER # Change USER's password ¹⁵ groups # List your groups ¹⁶ # If user is added into new group, changes will be effective since 17 # next login



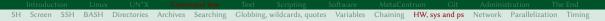
Users and groups

- These commands to manage users and groups do not have to work on all systems depends on authentication methods used
- Commands modifying users and groups require root authentication

```
# Add new user
<sup>2</sup> useradd new user name
   Modify user, see possible modifications
usermod --help
# Delete user
6 userdel user name
7 # Add new group
8 groupadd new_group_name
   Modify group, see possible modifications
10 groupmod --help
11 # Delete group
<sup>12</sup> groupdel group name
```

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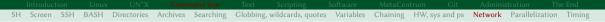


Tasks regarding hardware, information and processes

- 1 Change your password on the remote server and/or virtual machine.
- 2 Who is and was recently logged in to the remote server?
- **3** Which information about hardware can you get from your local computer (if you are running Linux) and from course server? Why could such information be useful?
 - Which disks are mounted?
 - 2 How many memory (RAM) slots are occupied and what is memory size?
- Find your user ID on local computer and remote server. Do you think this has any implications when copying files from your local computer to server and back?
- 5 Terminate from command line some running graphical application. What is difference between kill and killall?
- 6 Change priority of some running (graphical) application.
- Which applications are consuming the most resources (CPU, RAM)?

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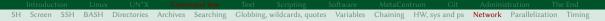
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Network protocols I

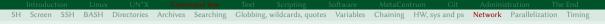
- Every network communication protocol (e.g. browsing web or Skype) has its own distinct port ("door to access target computer") it must be opened (by firewall)
- There are plenty of network services
 - Especially file servers and various data storages support more protocols to access the data according to operating system and/or use case
 - Sometimes it can be tricky to pick up (and configure) the right protocol
- SSH secure shell command-line connection to remote server to work there (port 22), slide 86
 - Plenty of other protocols can run over SSH (SFTP, SCP, SSHFS, rsync, ...)
- Telnet old deprecated insecure predecessor of SSH, never ever use it (port 23), only low-quality electronics still sometimes use it for administrative access
- FTP file transfer protocol outdated, no encryption (port 21), slowly replaced by FTPS (FTP secured) or SFTP/SCP (based on SSH)
 - Sometimes used only for download, e.g. ftp://ftp.ebi.ac.uk/pub/

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Network protocols II

- FTPS FTP with added connection encryption for higher security (port 21), common
- SFTP FTP over SSH common, secure (port 22), slide 139
- SCP secure copy uses SSH, but has restricted possibilities, common, secure (port 22), slide 139
- NFS network file share/server very common in UNIX world (commonly used e.g. by CESNET MetaCentrum and data storage česky), commonly used to permanently connect to network server, share directories, etc. (port 20049), slide 141
 - NFS connection must be set up by administrator
- webDAV file transfer over web (using WWW server) not so common, but good (port 80 or 443 same as WWW), slide 141
 - Accompanied by calDav and cardDav to share calendars and address books over the network
 - Used e.g. by ownCloud/nextCloud (also provided by CESNET česky) tool to synchronize and share files etc, similar to Dropbox, OneDrive or Google Drive
- SAMBA UNIX connection to Microsoft network shares (port 5445), slide 141



Network protocols III

- web "The Internet" for most of users (port 80 or encrypted 443)
- IMAP (port 143 or 993) and SMTP (port 25 or 465) to connect to e-mail server and send mails
- Messaging protocols like XMPP (Jabber), IRC, ICQ, MS Teams, Slack, Skype, ...
- Databases (if accessible over the Internet), and another special services, use to be available on dedicated ports
- And much more (see /etc/services)...
- Port number can be changed in configuration of respective server service
- All firewalls on the way must allow communication on given port some ports are commonly filtered in restrictive Wi-Fi networks or totalitarian countries

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Basic network information and testing

hostname # Get name of the computer ² ping web.natur.cuni.cz # Ping host. Is it alive? Cancel by Ctrl+C a traceroute www.metacentrum.cz # Get route (path) to the host 4 mtr seznam.cz # Combines ping and traceroute, quit with "q" ⁵ ip a s # Information about all network devices (MAC, IP address, ...) 6 ip r s # Show routes $_7$ # Does SSH work on the host? Verbose (-v), scan (-z), host, port number $_{8}$ # (22 for SSH, can be any) nc -vz web.natur.cuni.cz 22 ¹⁰ man nc # See for more information; "nc" is alias for "netcat" uss -atn # Information about all network connections 12 ss -ntplu # Show open TCP/UDP ports 13 ss -anp # Show active connections 14 ss --help # More options... ¹⁵ # If using nmap at faculty, firewall disconnects you for 10 minutes! 16 nmap -r someserver.cz # Scan someserver.cz for opened ports 17 nmap botany.natur.cuni.cz --script ssh-hostkey # See SSH key

Transferring files from/to remote server

- On server side, same files can be accessible (shared) by more methods
- **curlftpfs** allows mount FTP as local directory, but FTP is outdated, insecure and not constructed to that usage...
- wget https://some.address.cz/internet # Download file(s) from Internet wget --help # -r for recursive download (whole web), -k to convert links # curl is predecessor of wget, without parameter "-o" it prints remote curl https://some.server.cz/some/files -o localfilename # Copy files (-r for recursive) over SSH from local computer # to remote server or vice versa (just flip arguments) scp -r localfiles remoteuser@remote.server.cz:/remote/path/ scp -r remoteuser@remote.server.cz:/remote/files /local/directory/ # scp behaves like cp, but works over SSH
 - rsync is synchronization tool (commonly used for backups) able to connect to remote server (next slide)

Synchronization with rsync

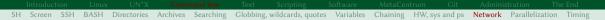
- rsync has huge amount of possibilities (see man rsync or rsync -h)
- Works locally as well as over network
- It transmits only changes very efficient
- Suitable for local as well as network backup
- Network address for rsync is written in same way as for scp
- --delete delete in target location files which are not in source location anymore
- --progress show progress percentage for every file
- --exclude=*.jpg
 skip JPG files
- For incremental backups use e.g. duplicity

rsync -arv somedirectory otherplace # All attributes, recursive, verbose

- 2 rsync -arv localdirectory user@remote.server.cz:/remote/directory/
- 3 rsync -arv user@remote.server.cz:/remote/data local/directory/

Connecting file systems on remote servers

- Target mount point must exist before mounting
- Servers can be accessed by IP address or hostname
- # Mounting remote server over SSH (sshfs package must be installed)
- sshfs USER@vyuka.natur.cuni.cz:/some/dir /local/mount/point
- 3 fusermount -u /local/mount/point # Disconnect SSHFS
- 4 # Mount Windows server (requires packages samba and cifs)
- 5 mount.cifs //windows.server.cz/Some/Directory /mnt/win -o \
 - credentials=/path/to/password.file,uid=USER,gid=GROUP
- 7 # "password.file" contains login credentials to Windows server:
- 8 username=user.name
- 9 password=TopSecretPassword1
- 10 domain=DOMAINNAME
- m # Mount NFS share (NFS is common protocol in UNIX world)
- mount -t nfs some.server.cz:/shared/directory /local/directory
- ¹³ # Mount webDAV folder (requires package davfs2 to be installed)
- mount -t davfs https://owncloud.cesnet.cz/remote.php/webdav/ /local/dir
- umount /mount/point # Disconnect CIFS/SAMBA, NFS, webDAV, ...



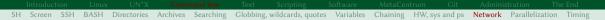
SSH keys I

Secure way how to connect to multiple servers with single key and more

- Secure way how to connect to multiple servers via SSH with single (or no) password using asymmetric encryption
- Command ssh-keygen generates pair of keys
 - Private key is typically in ~/.ssh/id_* file(s) (according to cipher)
 - Public key is typically in ~/.ssh/id_*.pub file(s) (according to selected cipher) and are copied to target servers
 - Private key is unlocked by password (might be without password) and it then allows to login to any server having the public key
 - Having only public key is not enough to login, private key without password is still not enough, but user must be sure private key is kept securely and not lost or stolen
 - When running it, ssh-keygen asks bunch of questions unless having special needs, keep defaults (hit Enter), using password for key is optional (but recommended)

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SSH keys II

Secure way how to connect to multiple servers with single key and more

- File ~/.ssh/known_hosts contain servers you have ever connected to, and their SSH fingerprints (unique IDs) if this changes, SSH complains a lot as it could be Man-in-the-middle attack
- File ~/.ssh/authorized_keys contains public keys allowing logging to the machine
- ~/.ssh/config can store various settings for particular servers
- SSH keys work in all applications using SSH (SFTP, SSHFS, rsync, Git, many graphical file managers, ...)
- User can have various local passwords on servers, but use single SSH key to connect to all of them, very convenient if connecting to multiple servers

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Connect to SSH with key

No need to remember password for every server...

```
# Create the key (several options)
<sup>2</sup> ssh-keygen -t rsa -b 4096 # Good security, portable
<sup>3</sup> # ECC gives better security, but not all servers/applications support it
4 ssh-keygen -t ecdsa -b 521 # Higher security
<sup>5</sup> ssh-keygen -t ed25519 # Same security as ecdsa, higher performance
6 # Empty (no) passphrase will connect to server without password
7 # Copy public key to remote server (private key must be kept locally)
8 ssh-copy-id user@remote.server.cz
• # Now, public key is on the server and private key in local computer is
<sup>10</sup> # unlocking the connection
" # Unlock the key (no need in some distributions or if there is no
<sup>12</sup> # passphrase) - must be done only once per user session
13 ssh-add
<sup>14</sup> # Connect as usually
```

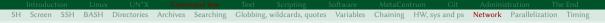
15 ssh user@remote.server.cz

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Network tasks I

- Create SSH key (if you don't have any), copy the public part to
 vyuka.natur.cuni.cz and connect there with SSH.
 - **1** What are advantages and disadvantages of having the key with or without password?
 - 2 Is there any reason for having multiple keys? Can you find any examples?
 - 3 Which services, protocols can use it? Find some examples.
- 2 Make in your notebook new empty directory and mount there via SSHFS your home directory on vyuka.natur.cuni.cz (or on some other server).
 - 1 Explore it. What is then path to files on the remote server?
 - Disconnect the server when done.
- 3 Use wget and curl to download this presentation to your notebook (link at slide 11).
 - For **curl** be aware of setting of output what is default behavior?
- Use scp to copy directory with toy data and scripts from your home directory on vyuka.natur.cuni.cz into your notebook.

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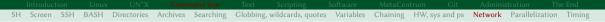


Network tasks II

- Subject to copy any file from your notebook into your home directory on vyuka.natur.cuni.cz.
- 6 Use rsync to update toy data and scripts in your notebook according to version on vyuka.natur.cuni.cz in /srv/scripts_data.
- Use rsync to update directory with toy data files and scripts in your home directory on vyuka.natur.cuni.cz according to version in your notebook.
 - For **rsync** try to use various options, run it several times.
 - Explore help of **rsync**. Can you find there some useful parameters?
- 8 Get MAC and IP address of your notebook. Why can be such information useful?
- 9 Ping some web server. Is it alive and well reachable?
- Why can be output of traceroute useful when you have problems with network?

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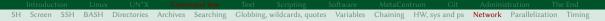
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Network tasks III

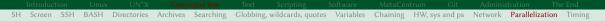
- Mount (explore and then unmount) your CESNET ownCloud into your notebook. If unsure, consult help (česky).
 - It is available for all academics in the Czech Republic, just go to https://owncloud.cesnet.cz and login with your institutional credentials
 - Alternatively connect to some other ownCloud/nextCloud/generic webDAV server
- What are advantages and disadvantages of mounting of remote servers (SSHFS, etc.) into local directories?
- Connect to vyuka.natur.cuni.cz (or any other server) using mc and copy there and back some files. What are advantages and disadvantages of mc when compared with usage of scp or rsync?
- Find in graphical interface of your computer how to connect via SSH/SFTP/SCP to transfer files. Connect to vyuka.natur.cuni.cz or some other server and transfer there and back some files.

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Faculty web server(s)

- Login requires same credentials as to CAS (login name, no ISIC number)
- Faculty information are only in Czech
- It is Linux server running Debian
- Connect with SSH/SFTP/SCP to web.natur.cuni.cz
- Mainly used for webhosting, user's address will have form
 https://web.natur.cuni.cz/~loginname/
 , user can apply for another
 URL, for space for some projects, ...
- Every department also has dedicated space there, it can be used for various web projects, address can be discussed with IT department
- Personal web can be placed in public_html within home folder
- Users can apply for MySQL database or special settings
- Department of Botany (and some other departments) have their own web and file servers



Parallelization with GNU Parallel

- GNU Parallel can distribute task among CPU threads of one computer, or even among different computers in network
- It is not (so) effective for short/small tasks
- Important operands (for more see man parallel and next slides)
 - {} input line whole line read from input source (typically standard input)
 - { . } input line without extension
 - {/} base name of input line only file name (without path)
 - {//} dirname from input line (filename is removed)
 - {/.} base name of input line without extension
 - ::: use arguments from command line instead of stdin (::: is placed after the command and before the argument)
 - :::: read from argument files
 - -j number of jobs if not provided, parallel will use all available CPU threads

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GNU Parallel examples I

```
# Convert all images from JPG to PNG
<sup>2</sup> find . -name '*.jpg' -print | parallel --bar convert {} {.}.png
# It might be possible to to use "'{}' '{.}.png'" instead
_{4} # Resize all images ("\" marks that command continue on next line)
5 find . -name '*.jpg' -print | parallel convert -resize 500x500 \
    -quality 75 '{}' '{.}-small.jpg' # or
7 parallel convert -resize 25% '{}' '{.}-small.jpg' ::: *.jpg
8 convert --help # See help of 'convert' from ImageMagick set
9 # Find WORD in huge text file (named "longfile" here) - this works
<sup>10</sup> # but it is not possible to get line number (file is red in blocks)
n parallel --pipe --block 10M -- grep --color=always WORD < longfile</pre>
12 nl longfile | parallel -k --pipe --block 20M -- grep WORD # Add line num.
<sup>13</sup> # When needed to get phrase or regular expression (use parameter
14 # "-q" for escaping of shell special characters or extra quotes):
<sup>15</sup> # "--" stops reading parameters for parallel
<sup>16</sup> nl longfile | parallel -qk --pipe --block 20M -- grep "WORD TEXT" # or
<sup>17</sup> nl longfile | parallel -k --pipe --block 20M -- grep ''WORD TEXT''
```

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GNU Parallel examples II

```
# Convert all WAV files into OGG
<sup>2</sup> parallel -X oggenc ::: *.wav # -X parse as many parameters as possible
<sup>3</sup> # Decompress all *.bz2 files in 'archive' directory using 2 CPU threads
4 parallel -j 2 -X bunzip2 -v ::: archive/*.bz2
<sup>5</sup> # Run in parallel commands from command list file (list of commands)
6 parallel < command_list.txt # (each command on one line) or</pre>
7 parallel :::: command list.txt
8 # Add same text to the end of multiple files
9 find . -name '*.txt' -print | parallel 'cat block_to_be_added.txt >> {}'
10 # Replace particular text in multiple files with sed and GNU Parallel
in find . -name '*.txt' -print | parallel 'sed -i "s/XXX/YYY/g" {}'
12 # Launch MrBayes for multiple nexus files and create log file with
<sup>13</sup> # starting and ending date and time
_{14} find . -name '*.nexus' -print | parallel 'echo -e "Start: (date) n" > \
15 {}.log && mb {} | tee -a {}.log && echo "End: $(date)" >> {}.log'
<sup>16</sup> # 'tee' copies output of the program into given log file
```

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GNU Parallel examples III and tasks

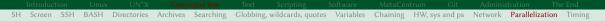
Create BCFtools statistics for all *.vcf.gz files
find . -name "*.vcf.gz" | parallel "echo '{/}' && bcftools stats -F \
reference.fasta '{}' > '{.}'.stats.txt"
Note that 'find' searches also in subdirectories
parallel --help # Basic help for GNU Parallel
man parallel # More information about GNU Parallel parameters

Tasks

- Resize using parallel photos foto_oxalis_*.jpg to 1000x1000 px.
- 2 Convert all above JPG files to PNG.
- Output Service Strain Strai
- **4** Think about some example solving your practical task where GNU Parallel would be helpful.

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Recording output of commands

- Alternative (commonly more convenient) to redirects of outputs to log file (slide 125) is command tee
 - · Very useful if redirects would be harder to code
- tee can record
 - All output of the software (standard as well as error output)
 - Commands (keys) typed by user it can be later reused to rerun the application unique feature useful for certain software

tee (-a for append to existing file) records output of any application command | tee record.txt # tee will record whole output of command tee record.txt | command # tee will record user input (NO command output) # If software reads commands from user, we can reuse record next time: command < record.txt # Empty lines are interpreted as Enter key # Each line is used whenever command waits for new # input (instead of typing, 'record.txt' is used)

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Launching of tasks at certain time

- at can run command at certain time (atd daemon must be running)
- Tasks are running in background, outputs are mailed (e.g. to /var/spool/mail/\$USER)

Check status of atd daemon (it must run), start/stop/enable/disable it ² systemctl status/start/stop/enable/disable atd.service a man at # Check for various possibilities of time settings at HH:MM # Run commands at certain time (hour:minutes) s at> command1 # Add as many commands as you wish (separate by Enter) 6 at> # When done, press Ctrl+D to cancel giving commands to at $_7$ # Instead of manual typing of tasks, run script at certain time & at HH:MM -f somescript.sh # Run somescript.sh at certain time ₉ at -1 # List of scheduled tasks (alias is atg) 10 at -r <number> # Cancel scheduled task (according to number from at -1) atrm # Alias for previous command 12 batch # Commands will be executed when system loads drops below 0.8 or 13

other value specified in configuration or startup of atd

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Automated launching of tasks

- cron runs tasks repeatedly (cron daemon must be running)
- Scripts for tasks running hourly/daily/weekly/monthly can be copied into respective /etc/cron.*/ directories
- Can be replaced by SystemD timers files (more complex, but more versatile)

```
# Check status of cron daemon (it must run), start/stop/enable/disable
<sup>2</sup> systemctl status/start/stop/enable/disable cron.service
3 crontab -1 # List user's cron tasks
4 crontab -e # Edit user's cron tasks (separate columns by spaces):
   Minute, Hour, Day in month, Month, Day in week, Command (absolute path)
   0-59
            0-23 1-31
                                 1-12 0-6 starting with Sunday (WTF?)
6 #
                                                      /usr/bin/command
    10
            22
                                              # 1st day in month, 23:11
            */3
    0
                                              # Every 3 hours
    0
            11
                                        0
                                              # Every Sunday, 12:00
10
    30
            3
                  * / 2
                                              # Every second day, 4:31
    */15
                                        0, 4
                                              # At Sun and Fri every 15 min
12
```

Reading	Extractions	AWK	Manipulations	Compressed text	Comj	parisons	Editors	Regular expressions	

Text

Various aspects of working with text files

5 Text

Reading Extractions AWK Manipulations Compressed text Comparisons Editors Regular expressions

Vojtěch Zeisek (https://trapa.cz/)	Linux, command line & MetaCentrum	January 14 to 16, 2025	156 / 317

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Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	

Everything is (text) file

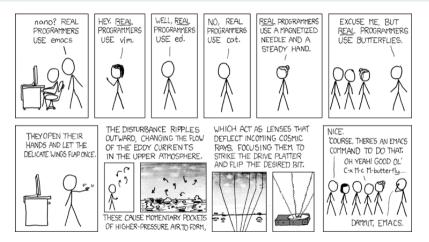
- As UNIX configuration and outputs (logs, ...) are mostly saved as relatively simple text files, manipulations of any type with text files is one of the most common tasks
 - Similar situation is for e.g. molecular data input/output data use to be text files with simple structure
- One of the most powerful features of BASH
- Some operations are complicated (e.g. complex manipulations with columns, various calculations) it is necessary to use AWK or Perl (probably the most advanced language working with text)
- Text-manipulating tools have very rich implementation of regular expressions (slide 191)
- Most of the operations are done in stream per line everything is very fast and memory efficient

Text tasks

Try all the commands from this chapter. It is one of key BASH features.

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	arisons	Editors	Regular expressions	

It is important to select good text editor ...



https://xkcd.com/378/

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	arisons	Editors	Regular expressions	

Importance of good text editor

Can your text editor ...?

- Show syntax highlight
- Show line numbers
- Show space between brackets
- Open any encoding and EOL
- Fold source code
- Show line breaks
- Mark lines
- Open multiple files
- Kate
- KWrite
- Vim

- GNU Emacs
- Geany
- Bluefish

- Advanced search and replace
- Use regular expressions
- Make projects, add notes
- Use command line
- Check spelling
- Debug source code
- And more...
- Gedit
- Notepad++
- Sublime

- VS Code
- Nano
- And more... = → <
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Reading	Extractions	AWK	Manipulations	Compressed text	Comp	arisons	Editors	Regular expressions	

Converting the text

Prevent bad display and weird errors when launching scripts

```
unix2dos textfile # Convert text file from UNIX to Windows EOL
unix2mac textfile # Convert text file from UNIX to old Mac EOL
dos2unix textfile # Convert text file from Windows to UNIX EOL
mac2unix textfile # Convert text file from old Mac to UNIX EOL
enca -h # See usage - enca converts various encodings (similar to iconv)
enca file.txt # Detects encoding of file.txt
renca -x utf8 file.txt # Convert file.txt into UTF-8
# Converts encoding of input file (ISO-8859-2) to outfile in UTF-8
iconv -f ISO-8859-2 -t UTF-8 infile.txt > outfile.txt
iconv -1 # List of available encoding to convert
```

- macOS uses same encoding and EOL as Linux (and rest of UNIX world), so there are no
 problems with compatibility
- Launching of bash script written on Windows on Linux/macOS will probably fail (because of different EOL)

Introduct									
Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	
Read	text file								

cat # Read or join (using redirects) files; 'cat --help' for options ² cat long text.txt # Print content of text file to the screen (stdout) a cat textfile1 >> textfile2 # Append textfile1 to the end of textfile2 4 nl long_text.txt # Like 'cat -n', prints textfile with line numbers 5 tac textfile # Like cat, but prints lines in reverse order 6 more long text.txt # When textfile is long, prints screen by screen # (space for next screen, q to quit) ⁸ # Better version of more - you can scroll up and down by PgUp, PgDown, 9 # arrows, searching by / (type searched string, hit Enter, n for next, 10 # twice ESC to quit), q to quit viewing (also used by man) 11 less long text.txt 12 fmt long text.txt # Basic formatting of text - joining of commented # lines, line breaks to break too long lines, ... 13 14 fmt textfile > formatted file # Save output of fmt into new file 15 wc long text.txt # Calculates lines, words and bytes in text file; 'wc -l' # for only lines, '-m' for characters, '-w' for words 16 $_{17}$ mc # It has text viewer (F3) and editor (F4)

```
Introduction Linux UN*X Command line Text Scripting Software MetaCentrum Git Administration The End
Reading Extractions AWK Manipulations Compressed text Comparisons Editors Regular expressions
```

Get part of text file (by lines) I

```
# head and tail are very convenient to quickly check file structure
<sup>2</sup> head -n N textfile # Print first N lines from textfile
a tail -n N textfile # Print last N lines from textfile
4 head -n-N textfile # Print textfile without last N lines
s tail -n+N textfile # Print textfile from Nth line to the end
6 # Split text file on selected pattern - creates new files xxXY
7 # Pattern can be regular expression - set it carefully
<sup>8</sup> # {*} says to repeat operation as many times as possible
g csplit textfile '/pattern/' '{*}' # pattern itself is inside '/___/'
<sup>10</sup> # Split text file by lines into multiple files
\mu # e.g. suffix will be of length 5 (-a 5), suffix will be numeric (-d),
12 # list.txt will be split every 10 lines (-1 10) and output names will
" # start by 'lists_'
14 split -a 5 -d -l 10 list.txt lists_
split -t ... # Split by separator, not by newline
<sup>16</sup> # Both csplit and split are very versatile, see their help
```

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	

Get part of text file (by lines) II

- grep --help # See plenty of options
- ² grep -parameters pattern textfile # Write lines containing pattern
- ³ grep user /etc/passwd # Write all lines in passwd file containing "user" 4 cat /etc/passwd | grep user # Same as above, common, but superfluous style 5 grep -v user /etc/passwd # Write all lines in passwd NOT containing "user" 6 grep -c user /etc/passwd # Get number of lines in passwd containing "user" 7 grep -i USER /etc/passwd # -i for case insensitive
- 8 grep -q ... # quiet no output (only T/F) good for testing in scripts 9 grep -ls user /etc/* # -l print files with pattern, -s suppress errors 10 grep "longer text" textfile # Extract whole phrase (must be quoted)
 - Grep supports regular expressions, slide 191
 - Grep works per-line, multiline patterns are more or less impossible (use AWK or Perl instead) this is general limitation of basic tools
 - Grep (and sed and other tools) in macOS is outdated, missing plenty of functions use version from Homebrew (slide 80)

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Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	

Work with columns

- cut extracts columns, paste joins, column reformates
- BASH can not select column according to its name (Perl can do that)
- cut column/delimiter+field textfile
- 2 cut -c 1 /etc/group # Get first character
- 3 cut -c 1-5 /etc/group # Get character 1-5
- $_{\rm 4}$ cut -c 4- /etc/group # Get character 4 and more
- 5 cut -c 2,5,7 /etc/group # Get characters 2, 5 and 7
- 6 cut -d ':' -f 1 /etc/group # Select 1st field separated by ":"
- 7 cut -d ':' -f 2-4 /etc/group # Select fields 2-4 separated by ":"
- 8 cut -f 1,2 cut_awk_test_file.tsv # get columns 1 and 2 separated by TABs
- 9 # Add second file as second column
- paste file1 file2 > outputfile
- $\scriptstyle\rm II$ # Output will be two columns (from file1 and file2) separated by TAB
- 12 paste -d "|" diff_test_file_1.txt diff_test_file_2.txt # -d for delimiter
- ¹³ # Swapping columns is not very comfortable...
- 14 paste <(cut -f 2 cut_awk_test_file.tsv) <(cut -f 1 cut_awk_test_file.tsv)</pre>
- 15 ls -1 | column -t # Reformate input as table (compare with 'ls -l')

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	arisons	Editors	Regular expressions	

Examples of usage of head, grep and cut with our data I

- head long_text.txt # Beginning of the file
- ² # Extract names of FASTA sequences
- 3 grep "^>" Oxalis_HybSeq_nrDNA_selection_alignment.fasta
- 4 # How many sequences are there?
- 5 grep -c "^>" Oxalis_HybSeq_nrDNA_selection_alignment.fasta
- 6 # Extract every FASTA sequence containing "AAAAAA" and name of
- 7 # respective FASTA sequence
- 8 grep -n -B 1 AAAAAA Oxalis_HybSeq_nrDNA_selection_alignment.fasta
- 9 # Get column of pairwise identities of sequences exported as TSV from
- ¹⁰ # Geneious discard header (1st line, print from 2nd line) and extract ¹¹ # second column (separated by TAB)
- 12 tail -n+2 cut_awk_test_file.tsv | cut -f 2 | less
- 13 # Number of occurrences of word "Gregor" in file long_text.txt
- 14 grep Gregor long_text.txt | wc -1 # Number of matching lines
- 15 grep -c Gregor long_text.txt # Number of occurrences
- 16 ls -1 *.sh | wc -1 # How many BASH script are in current directory

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Examples of usage of head, grep and cut with our data II

Extract from FASTA only sequence names into names.txt
grep "^>" Oxalis_HybSeq_nrDNA_selection_*.fasta | sed 's/^>//' > names.txt
Save names of oxalis* JPG files into list_oxalis_photo.txt and see it
4 ls -1 *oxalis*.jpg > list_oxalis_photo.txt && cat list_oxalis_photo.txt

Tasks

- How many samples of Oxalis hirta are in Oxalis_HybSeq_nrDNA_selection_alignment.fasta?
- From Oxalis_HybSeq_nrDNA_selection_alignment.fasta extract only sequences of Oxalis hirta and save them into oxalis_hirta.fasta.
- From Oxalis_HybSeq_nrDNA_selection_alignment.fasta extract only sequences of Oxalis amblyosepala and O. gracilis and save them into oxalis_spp.fasta.

Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	

Get a column with awk

- AWK is scripting language mainly for text manipulations
- Can do things other BASH tools can not (easily) do better manipulation with columns, calculations, work with multi-line patterns, ...
- Has complicated syntax, it is hard to read, it is not similar to other tools Perl can do more and is more common (learn it instead)...
- Supports regular expressions, slide 191
- Can not select column according to its name (Perl can do that)
- For more information see manuals https://www.gnu.org/software/gawk/manual/, https://en.wikibooks.org/wiki/An_Awk_Primer and https://www.grymoire.com/Unix/Awk.html

awk 'regexp { commands parameters }' file # General syntax

• = •

Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	

AWK examples I

```
# Print last column (separated by tab, built-in variable $NF)
<sup>2</sup> awk '{print $NF}' cut awk test file.tsv
# Select 2nd column ($2; separated by tab)
4 awk '{print $2}' cut_awk_test_file.tsv
<sup>5</sup> # Print columns 3 and 2 (in this order)
6 awk '{print $3, $2}' cut awk test file.tsv
7 # Get column 5 and 1 (in this order, separated by ":") from /etc/passwd
8 # (only lines containing "home") print ", username:" between the columns.
• # Note usage of commas and consequences to output.
prep home /etc/passwd | awk -F ':' '{print $5 ", username:", $1}'
" # Separate columns by TAB, /^d/ for lines starting with "d" (only dirs)
12 ls -1 | awk '/^d/ { print $8 "\t" $3 }'
<sup>13</sup> # Print on even lines ">", former column 1, new line, former column 2:
14 # 2 columns into 2 lines (create FASTA from tabular record)
awk '{print ">"$1"\n"$2}' awk_test_file.tab | less -S
_{16} # Print field 1, TAB (\t), length of field 2, TAB and field 2
awk '{print $1"\t"length($2)"\t"$2}' awk test file.tab
```

Reading	Extractions	AWK	Manipulations	Compressed text	Com	iparisons	Editors	Regular expressions	

AWK examples II

If field (column) 2 contains exactly 100.0%, print whole line (\$0) ² awk '{if(\$2=="100.0%"){print \$0}}' cut awk test file.tsv # Field 1 is numeric (less then 5 digits) - add leading zeroes awk '{printf "05d', \$1;}' awk test file.tab 5 # As previous, but add leading zeroes to field 1 and print whole line awk '{\$1=sprintf("%05d", \$1); print \$0}' awk test file.tab 7 # Field 6 is numeric, select lines where field 6 is higher than 200 8 awk -F '\t' '\$6>200' cut_awk_test_file.tsv # Separated by TABs (\t) 9 # Print fields 4 and 5 (fields are separated by " " or TAB) ward awk -F '[\t]' '{print \$4, \$5}' cut awk test file.tsv " # Precede each line by its line number for all files together, with TAB $_{12}$ # (i.e. print line number (NR) and then whole original line (\$0)) 13 awk '{print NR "\t" \$0}' diff_test_file_* ¹⁴ # Substitute "a" with "XXX" ONLY for lines which contain "the" 15 awk '/the/{gsub(/a/, "XXX")}; 1' diff test file 1.txt

Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	

AWK examples III

For every 4th line starting from line 2 of FASTQ file (from line 2
every 4th line contains the DNA sequence) print its length (bzcat
prints content of file compressed by bzip2)
bzcat Oxalis_hirta_R1.fastq.bz2 | awk 'NR%4==2{ print length(\$0) }'
If sequence is longer that 500 bp (length of field 2), print its name
(field 1) like this "Seq. name: TAB the sequence name (ID)"
awk '{if(length(\$2)>500){print "Seq. name:\t" \$1}}' awk_test_file.tab
Extract from awk_test_file.tab sequences over 500 bp, sort theme by name
and save them as FASTA file
awk '{if(length(\$2)>500){print \$0}}' scripts_data/awk_test_file.tab | \
sort -n | sed 's/^// | sed 's/[[:blank:]]\+/\n/g' > 500bp.fasta

Introduct									
Reading	Extractions	AWK	Manipulations	Compressed text	Comp	arisons	Editors	Regular expressions	
Sortin	σl								

sort file # Sorting is influenced by locale setting (e.g. Czech "ch") ² LC ALL=C sort ... # To force use of English locale use # Take into account only spaces and alphanumerical characters (ignore ₄ # any other) ⁵ sort -d textfile # Only spaces and alphanumerical characters 6 sort -r textfile # Reverse order 7 sort -f textfile # Ignore character case (not case sensitive) 8 sort -m textfile1 textfile2 # Merge already sorted text files 9 sort -u textfile # Print only first of multiple (repeated) entries ¹⁰ # Extract only unique sequences from FASTO bzcat Oxalis hirta R1.fastq.bz2 | awk 'NR%4==2{print \$0}' | sort -u ¹² sort -b textfile # Ignore leading blanks (space on beginning of line) 13 sort -k 2 -n cut_awk_test_file.tsv # Sort according to 2nd field 14 # Filters following identical lines - only unique are printed unig textfile 16 sort textfile | uniq # To get unique lines from whole file, sort it first

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Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	
Sortin	g								

```
uniq -c textfile # Add number of occurrences before each line
<sup>2</sup> unig -d textfile # Print only repeated lines
unig -i textfile # Ignore case (not case sensitive)
4 uniq -s N textfile # Skip first N characters
s uniq -u textfile # Print only not-repeated lines
6 # How many times is each taxon presented in
7 # Oxalis HybSeq nrDNA selection alignment.fasta
a grep -o "Oxalis [a-z]+" Oxalis HybSeq nrDNA selection alignment.fasta
9
      sort unig -c sort -r
10 # Find sizes of directories in /home (ignore errors caused by restricted
# permissions) and sort output according to sizes
_{12} du -sh /home/* 2>/dev/null | sort -h | sed 's/\/home\///'
<sup>13</sup> # Sort *.sh scripts according to number of lines
wc -1 *.sh | head -n-1 | sort -bn
```

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Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	

Replacements with tr

• tr replaces or deletes characters from standard input and writes result to standard output — use pipes and/or redirects

```
# Replace space by TAB in inputtextfile, save result as outputtextfile
2 cat inputtextfile | tr " " "\t" > outputtextfile
# Delete "text" from each line and print it to standard output (screen)
a cat inputtextfile | tr -d "text"
_{5} # Replace every occurrence of A, B, C or D by a new line (\n)
6 cat inputtextfile | tr "[ABCD]" "\n" > outputtextfile
7 # Replace capital letters by small ones
% tr "[A-Z]" "[a-z]" < diff test file 1.txt > outputtextfile.txt
# Alternative (easier reading) of previous command:
to cat diff test file 1.txt | tr "[:upper:]" "[:lower:]" > outputtextfile
# Replace all new lines (line breaks) by TABs
_{12} cat diff test file 1 | tr "\n" "\t" > outputtextfile
<sup>13</sup> # Discard all new lines - output will be one line
_{14} tr -d "\n" < textfile > /dev/stdout # stdout is typically screen
15 tr --help # See another possibilities for pattern to find/replace
```

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	arisons	Editors	Regular expressions	

Replacements with sed

- sed supports regular expressions, see slide 191 (same as in grep and vim), with parameter -r can use extended regular expressions (do not confuse the syntax is slightly different, richer)
- Output is written to standard output use pipes, redirects or -i to modify the file in place (without printing of output)
- macOS has old outdated versions of grep, sed and other tools (richness of regular expressions is poor) use versions from Homebrew (slide 80) or search Internet how to modify the patterns...
- Option -S separates multiple files (otherwise lines in multiple files are calculated as one stream)
- Option -n use to be used when deleting lines or printing only specific lines to suppress other lines (see examples)
- See manuals https://www.gnu.org/software/sed/manual/ and https://www.grymoire.com/Unix/sed.html

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Sed examples I

• Various parameters, modificators, operators can be combined...

```
sed 'operator/FindToReplace/Replace/modificator' textfile > newtextfile
<sup>2</sup> # Search and replace ("s") all occurrences ("g") of "find" by "replace"
<sup>3</sup> sed 's/find/replace/g' textfile
<sup>4</sup> # Replace third occurrence of pattern on every line
s sed 's/pattern/Replace/3' # 's/.../3' replace only third occurrence
6 sed '1,7s/...' # To work only on particular line, place single number or
_7 sed '5s/...' # range (e.g. 1,7) right before "s" ("$" for last line)
<sup>8</sup> sed '1~2n;s/F/R/g' # Work on every second line, starting by line 1
9 sed -n '2~10p' # Print every 10th line, starting with line 2
10 \text{ seg 1 } 100 | \text{ sed -n '} 2 \sim 10p' \# \text{ Example of above pattern (see "seg 1 100")}
\mu # Replace first TAB (\t) on each line by new line (\n)
_{12} sed 's/(t/n)' textfile
13 # Convert sequences in tabular format into FASTA (place ">" to the
<sup>14</sup> # beginning of the line, replace TAB "t" by newline "n")
_{15} sed \frac{s}{1}/\frac{s}{1} awk_test_file.tab | sed \frac{s}{1}/\frac{t}{n'} seq.fasta
```

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Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	
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Sed examples II

Convert FASTO sequences into FASTA (on every 4th line, starting with ² # line 1 replace "@" by ">", print every 4th line, starting by line 2) 3 bzcat Oxalis hirta R1.fastq.bz2 | sed -n '1~4s/^@/>/p;2~4p' > seq.fasta 4 sed -i 's/find/replace/g' directory/* # Process all files in directory 5 # Convert all capital letters into lower 6 sed 's/[A-Z]/\L&/g' inputtextfile > outputtextfile # And vice versa: $_7$ sed 's/[a-z]/\U&/g' inputtextfile > outputtextfile ⁸ # Groups to remember work in same way in sed, grep as well as vim: $_{9}$ # \(ToRemember\) # Remember expression in brackets and then use 10 # Number # Use remembered expression (numbered from one: 1, 2, 3, ...) " # Take output of 1s -1 and replace value of \$USER by "\$USER-RULEZZZ" 12 ls -1 | sed "s/\(USER)/\1-RULEZZZ/g" # Note " to use the variable ¹³ # Replace size column (2nd numeric) by "size:TAB<file size>b" ¹⁴ # Second sed replaces any white spaces by single TAB 15 ls -1 | sed 's/([0-9]+)/size:(t)/1b/2' | sed 's/[[:blank:]]+/(t/g')16 sed '/^\$/d' long text.txt | less # Delete blank (empty) lines head long text.txt | sed '6d' # Delete 6th line

Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	

Sed examples III

sed 's / * / ' # Delete extra spaces on the end of lines² sed '/GUI/d' # Delete all whole lines containing "GUI" ³ sed 's/GUI//g' # Delete all occurrences of "GUI" (not whole lines) 4 sed '4 i\Linux is great.' diff test file 1.txt # Insert to 4th line sed '3 a\Linux is great.' diff_test_file_1.txt # Insert after 3rd line 6 # Insert text to the beginning of the 3rd line (compare with previous) $_7$ # "^" is beginning of line, \$ end ('\$/...' last line) 8 sed '3s/^/INSERT/' diff test file 1.txt 9 # From ls -1 keep number of links (1st numeric column after permissions) ¹⁰ # and then flip user and group and print it as "group:user" n ls -1 | sed 's/ \([[:digit:]]\+\) \([[:alnum:]]\+\) \([[:alnum:]]\+\) / 1_2 $1_3: 2 / g' \#$ Note separating spaces (previous line ends with space) 13 1s -1 # Compare to the previous command, explain behavior of sed pattern 14 # Escaping - replace dot by comma (dot means any single character) $_{15}$ sed 's/\./,/g' diff_test_file_1.txt # \ escapes following character $16 \text{ sed } \frac{s}{...,g}$ diff test file 1.txt # Compare with the previous example

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Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	

Sed examples IV

```
# Replace any of characters within [...] by some pattern
_{2} sed 's/[abcd]/X/g' diff test file 1.txt # Compare with reverse case:
3 sed 's/[^abcd]/X/g' diff test file 1.txt # "[^...]" means anything else
4 sed -i ... file.txt # In-place editing - file is edited, no output to
                      # standard output (no need for redirects and pipes)
6 ls -1 | sed 's/[0-9]\{4,\}/BIG!/' # Replace 4 or more digits by "BIG!"
7 sed -E ... sed -r ... # Use extended regular expressions (see further)
<sup>8</sup> # Remove blank space (spaces or tabs) on beginning of each line
sed 's/^[[:blank:]]\+//' textfile
<sup>10</sup> # Remove suffix from names of *.sh files - compare variants
1 ls -1 *.sh | sed 's/\.sh$//' # Note '$' to ensure end of line
12 ls -1 *.sh
_{13} find . -name "*.sh" | sed 's/\.///;s/\.sh//' # Note chaining of patterns
14 find . -name "*.sh" # It searches also in subdirectories
```

Sed does not perform well on multi-line patterns — better is to use AWK or Perl

Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	

Joining

- Generally, most of tools work per-line, paste appends columns (see also slide 164)
- **join** compares every matching lines (by default 1st field) and creates all combinations ensure to have sorted input files with unique text
 - E.g. if 1st file contains A B and A C and 2nd file A D and A E, the result will be A B D, A B E, A C D and A C E

```
# Add file to the end of another text file
cat file1 >> file2 # file2 will contain both files, file1 is unchanged
# Compare two sorted text files and write shared lines
# (duplicitous lines are shown just once)
join textfile1 textfile2 > outputfile
# If used on wrong files, it can create huge file
seq -f "1 %g" 100 > aaa && less aaa
seq -f "1 %g" 100 > bbb && less bbb
join aaa bbb | wc -l
join --help # See more options...
```

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Variants of basic commands for processing of compressed text files I

- Many tools are able to directly handle files (i.e. single text files) compressed by gzip
- For files compressed by gzip use zcat (instead of cat), zdiff (instead of diff), zegrep (instead of egrep), zfgrep (instead of fgrep), zless (instead of less), zmore (instead of more), ...
- For files compressed by bzip2 use bzcat, bzdiff, bzegrep, bzfgrep,
 bzless, bzmore,...
- For files compressed by 1zma or 1zma2 (xz, 1zma) use 1zcat, 1zdiff, 1zegrep, 1zfgrep, 1zgrep, 1zless, 1zmore,...
- Sometimes these variants are used automatically when user works with compressed file
- mc can also do the job
- These tools sometimes don't have all options of the "standard" applications
- Scientific data formats are often compressed by GZIP (FASTQ, VCF,) ,

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s://trapa

Linux, command line & MetaCentrum

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	

Variants of basic commands for processing of compressed text files II

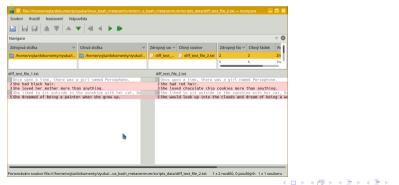
- # Extract lines with grep zgrep FORMAT arabidopsis.vcf.gz # 'less -S' displays long lines without indent (use R/L arrows to move), # zless doesn't have such option - use as follows: zcat arabidopsis.vcf.gz | less -S # zless doesn't have the -S option... # Display file compressed by bzip2 bzless Oxalis_hirta_R2.fastq.bz2 # Get end of the file bzcat Oxalis_hirta_R2.fastq.bz2 | tail # Get number of lines bzcat Oxalis hirta R2.fastq.bz2 | wc -1
 - Not all commands to work with text have variant to work with compressed files...
 - Variants to work with compressed files sometimes don't have all options...
 - Sometimes it's the best to pipe zcat / bzcat and another tool

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Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	

Comparisons

- Graphically compare two files by e.g. Kompare, DiffMerge, Meld, ...
- Most common is usage of GNU diffutils (next slide), see manual https://www.gnu.org/software/diffutils/manual/
- See also guide with examples, česky příklady na diff a porovnání dvou textových souborů



Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	
	1 1.0	c							
comm	n and dif	t							

```
cat diff_test_file_1.txt diff_test_file_2.txt # See and use examples
<sup>2</sup> # Compare two sorted columns: 1st column - lines only in textfile1; 2nd
<sup>3</sup> # column - lines only in textfile2; 3rd column - lines in both files
a comm textfile1 textfile2
_{5} # Don't show 2nd column (similarly -1, -3)
6 comm -2 diff test file 1.txt diff test file 2.txt
7 # Show differences between text files
8 diff diff test file 1.txt diff test file 2.txt
   # First number shows line(s) in 1st file, then if add/delete/change
   # and last number shows line(s) in the second file, <> show direction
10
u diff -e diff test file 1.txt diff test file 2.txt # More simple output
12 diff -c diff test file 1.txt diff test file 2.txt # Show context
B diff -u diff test file 1.txt diff test file 2.txt # Better, most common
14 diff -y diff test file 1.txt diff test file 2.txt # In two columns
15 colordiff # Same usage and parameters as previous, colored output
16 colordiff -u diff test file 1.txt diff test file 2.txt # Most common
```

Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	

diff and patch

- Users of vim (slide 188) can display the diff in vim, or use vimdiff
- In vimdiff swap between panes by Ctrl+W+W
 - Can open more files, works like standard vim (from slide 188), individual files can be saved

```
# Display diff in vim
```

```
<sup>2</sup> diff -u diff_test_file_1.txt diff_test_file_2.txt | view -
```

```
_{\rm 3} # vimdiff can show more colors, launches vim (exit by <ESC>:q!<Enter>)
```

4 vimdiff diff_test_file_1.txt diff_test_file_2.txt

- Saves difference between two files it can be later used as template to modify original file
- Single patch file can contain changes from multiple files
- Patch file from diff -u is common way how to send changes, improvements, ...
- # Create the diff file use like "diff old new"
- 2 diff -u diff_test_file_1.txt diff_test_file_2.txt > difference.diff

```
<sup>3</sup> # Apply the patch - xxx_file_1.txt is patched according to xxx_file_2.txt
```

- 4 patch < difference.diff # or</pre>
- 5 patch diff_test_file_1.txt difference.diff

Reading	Extractions	AWK	Manipulations	Compressed text	Comj	parisons	Editors	Regular expressions	

Command line text editors

- nano, pico and mc are very simple, just for very basic text editing in command line or until you learn vim (graphical version is gVim) or emacs (graphical versions are also available, just search for Emacs in your distribution software manager)
- You can work most of the time in graphical editors (slide 159)
- Emacs and Vim are extremely rich, but having completely different approach when you get use to one, you can't use the another

• Task: Run vimtutor and follow instructions there.

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Reading	Extractions	AWK	Manipulations	Compressed text	Comp	arisons	Editors	Regular expressions	

The editors and their usage

- In nano and pico see bottom line for commands
 - Ctrl+O to write the file, Ctrl+X to guit the editor, Ctrl+G for help (^ stands for Ctrl kev)
- In mc highlight the file to edit and press F4
 - F2 to save, F10 to quit, F1 to help, F9 for top menu (navigate with arrows, cancel with double **Esc**), it is possible to use mouse
- **Emacs** use huge number of commands with **Ctrl** key (basics on next slide)
 - See https://www.gnu.org/software/emacs/tour/, https://tuhdo.github.io/emacs-tutor.html and https://systemcrafters.net/emacs-essentials/ absolute-beginners-guide-to-emacs/
- The most common (but very complex and specific) is Vim
 See https://vim-adventures.com/ to play a game and learn Vim (and derivatives)
- Emacs and Vim have huge number of possibilities and support for plugins and scripts, but completely different usage style - one person can really learn only one...
- If regularly working in command line, master any command line editor

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	

Emacs basics

- Feature-rich ecosystem not only text editor, also file manager, debugger, integrated development environment, extra plugins are available, ...
- Keyboard commands are noted as e.g. C-x, where "C" stands for (mostly) Ctrl key, M-x, where "M" stands mostly for Alt key (Meta), sometimes for Win key
- C-h C-h help (twice Ctrl + H)
- C-x C-c quit (X-g for particular buffer, etc.)
- C-x C-f open file
- C-x C-s save file
- C-x C-w save file as
- C-_ undo
- C-s search forwards

- C-r search backwards
- C-left move one word left
- C-right move one word right
- C-up move one paragraph up
- C-down move one paragraph down
- M-% search and replace pattern

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Reading Extractions AWK Manipulations Compressed text Comparisons Editors Regular expressions											
	Rea	ding B	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	

Vim

Vim has three different working modes

- **Normal**" nothing is displayed in bottom left corner, every key has some meaning (next slide) very powerful manipulations with text
 - i or Insert key to enter *insert mode*, : to enter *command mode*
- Insert in bottom left corner " -- INSERT -- " is displayed, the most familiar mode, normal typing etc., exit to normal mode by ESC key
- Command in bottom left corner : is displayed, awaits commands, exit to normal mode by Backspace key (delete ": ")
- See documentation https://vim.fandom.com/wiki/Vim_Tips_Wiki, https://www.vim.org/docs.php;česky https://www.nti.tul.cz/~satrapa/docs/vim/
- For interactive learning try https://vim-adventures.com/ (Task: Play it for a while.:-) or command vimtutor

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Normal and command Vim modes

• Normal mode (press ESC)

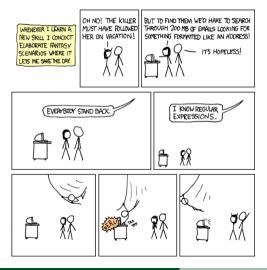
- dd cut current line
- **r** replace single character below cursor (type then character to be placed instead of the original one)
- v for selection of text (and then e.g. delete by d or copy by y)
- y copy selection
- x cut selection (always to clipboard, it can be pasted by p)
- p paste
- *number* to get to line of particular line number
- u to undo last change(s)

- /ToSearch search "ToSearch" (once press Enter, n for next occurrence, quit with Esc)
- Command mode (press ESC :)
 - w write file
 - q quit
 - **q**! quit and discard changes
 - <mark>%s/...</mark> to search and replace as in sed
 - syntax on/off turn syntax highlight on/off
 - set nu show line numbers

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Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editor	5	Regular expressions	

Regular expressions are useful...



- Find text according to a pattern
- Manipulate the text flip, reformat, replace, ...
- Syntax is variable among programming languages and applications
- There are commonly more solutions for one task
- Well supported in grep, sed, awk, vim, emacs, ...
- Probably the most advanced is Perl
- Implementations can differ among tools

https://xkcd.com/208/

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	

Regular expressions I

- Implementation in vim, sed, grep, awk and perl and among various UNIX systems is almost same, but not identical can be confusing...
- grep, sed and vim require escaping of +, ?, $\{$, $\}$, (and) by backslash \setminus (e.g.
 - +, see also next slides)
 - These characters have special meaning (see further) consider if you search for e.g. literal + or not (and then you can use it's special meaning)
- egrep (extended version, launched as grep E ... or egrep ...), sed with extended reg exp (sed -r) and perl do not require escaping (simply just e.g. +, not \+)
- Mastering regular expressions require practicing solve practical problems and see their power
- Read https://en.wikibooks.org/wiki/Regular_Expressions, https://www.grymoire.com/Unix/Regular.html, https://www.regular-expressions.info/

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	

Regular expressions II

- Česky https://www.nti.tul.cz/~satrapa/docs/regvyr/, https://www.root.cz/serialy/regularni-vyrazy/ ahttps://www.regularnivyrazy.info/
- Manuals for Grep, Vim, Sed, Awk, Perl (newer Perl 6 Raku), ...
- See sed examples, slide 175; and next slides
- macOS has by default very outdated version of sed and another tools it does not have all advanced features — users need to install e.g. gnu-sed formulae from Homebrew (slide 80), similarly for Grep, AWK, ...
- Do not confuse with shell globbing (slide 110) regular expressions are used withing particular application (GNU Sed, GNU Grep, Perl, ...), while shell globbing is in-build BASH feature
 - Globbing as well as regular expressions match/expand particular text string (in case of globbing typically file names)

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Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	

Regular expressions III

- Regular expressions mostly must be quoted ('...') **not** to be interpreted by shell, they work mostly with **text** files (their versatility allows to use them to work with e.g. molecular data)
- Word processors (LibreOffice, ...), graphical text editors, etc. usually also support regular expression, more or less following syntax below, but sometimes bit simplified
- _ _ _ any single character
- * any number of characters/occurrences of pattern (including 0)
- + one or more occurrences of the preceding reg exp
- ? zero or one occurrences of the preceding reg exp
- [...] any character in the brackets (can be list like [abcd] or range like
 [a-kxz4-8_-])
- [^...] reverse case all characters except newline and those listed in brackets

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Reading	Extractions	AWK	Manipulations	Compressed text	Com	parisons	Editors	Regular expressions	

Regular expressions IV

- \land first character of reg exp beginning of the line
- \$ last character of reg exp end of the line
- $\{n, m\}$ range (number) of occurrences of single character (from *n* to *m*)
- $\setminus \{n \setminus \}$ exactly *n* occurrences
- $\setminus \{n, \setminus\}$ at least *n* occurrences
- \ escape following special character (e.g. \. to literally search for dot and not "any single character")
- | either the preceding or following reg exp can be matched (alternation), in grep etc. escape it and use as \|

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	arisons	Editors	Regular expressions	

Regular expressions V

- (...) remembered group reg exp (numbered, starting with 1) can be called by n, where *n* is number of the group (starting with 1, see examples further)
- $\backslash <$, $\backslash >$ word boundaries
- [[:alnum:]] alphanumerical characters (includes white space), same like
 [a-zA-Z0-9]
- [[:alpha:]] alphabetic characters, like [a-zA-Z]
- [[:blank:]] space and TAB
- [[:cntrl:]] control characters
- [[:digit:]] numeric characters, like [0-9]
- [[:graph:]] printable and visible (non-space) characters

Reading	Extractions	AWK	Manipulations	Compressed text	Comj	parisons	Editors	Regular expressions	

Regular expressions VI

- [[:lower:]] lowercase characters, like [a-z]
- [[:print:]] printable characters (includes white space)
- [[:punct:]] punctuation characters
- [[:space:]] white space characters
- [[:upper:]] uppercase characters, like [A-Z]
- [[:xdigit:]] hexadecimal digits
- ^\$ blank line
- ^ . * \$ entire line whatever it is
- + one or more spaces (there is space before plus)
- & content of pattern that was matched

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	

Grep and sed examples I

• Be sure to understand all syntax on this and following slide...

```
# Extract sequences with at least 5 A bases in line
_{2} grep "A\{5,\}" Oxalis HybSeq nrDNA selection alignment.fasta
<sup>3</sup> # Extract DNA sequence string ATCG or ATGC
4 grep "ATCG\|ATGC" Oxalis_HybSeq_nrDNA_selection_alignment.fasta
# Get guality of Illumina reads mapping to reference in genomic VCF
6 zcat arabidopsis.vcf.gz | grep -o "MO=[[:digit:]]\+" | sed 's/^MO=//'
7 # How many times there is a direct speech (text between "...")
grep -o '"[[:upper:]][a-zA-Z0-9,\.\?\! ]\+"' long text.txt | wc -1
• # Add after dot on the end of the line by extra line break
sed \frac{s}{\sqrt{n'}} long text.txt | less
\pi # Add HTML paragraph tags ( and )
12 \text{ sed } -e \frac{s}{\sqrt{p}}' -e \frac{s}{\sqrt{p}}' \log \text{ text.txt} less
<sup>13</sup> # Make first word of every paragraph bold in HTML (<strong>...</strong>)
_{14} sed -e 's/^/<strong>/' -e 's/^[[:graph:]]\+/&<\/strong>/' long text.txt
```

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	

Grep and sed examples II

How many times is each word in the text ² grep -o "\<[[:alpha:]]\+\>" long text.txt | sort | uniq -ic | less a # List all Internet web links a grep -o 'https?://[a-zA-Z0-9].()/:]+' long text.txt5 # Convert selected letters to upper case 6 sed 's/[acegikmoqsuwy]/\U&/g' diff_test_file_1.txt $_7$ # From file listing (compare with 'ls -l') remove permissions and number ⁸ # of links on the beginning, flip user and group ownership and add labels 9 # Note usage of numbered groups ¹⁰ # Note that unmatched part o line is intact 1 1s -1 | sed 's/^[[:graph:]]+[[:blank:]]+[0-9]+[[:blank:]]+ $\frac{12}{([:alnum:]]+)[:blank:]]+([[:alnum:]]+)/GRP: \2\tUSR: \1/g'$ ¹³ # Create list of samples (e.g. as input in script for some application) $_{14}$ SAMPLESLIST= $(find . -name "*.jpg" | sed 's/\.\///' | sed 's/^/-I /'$ tr "\n" " ") 15 16 echo \$SAMPLESLIST # What would be difference from quoted "\$SAMPLESLIST"? 17 application \$SAMPLESLIST -method X -out Y ... # Rationale of such listing

Reading	Extractions	AWK	Manipulations	Compressed text	Comp	parisons	Editors	Regular expressions	

Regular expressions tasks

- Remove "S" codes, replace underscore by dot and space (...), and capitalize initial "o" in FASTA names in oxalis_assembly_6235.aln.fasta, e.g. from >o annae S499 to >O. annae.
- Extract from arabidopsis.vcf.gz values of DP (only numbers), sort them and print on single line, separated by commas.
- Otermine, which sequence(s) of Oxalis_HybSeq_nrDNA_selection_alignment.fasta has block of missing data (N) or spaces (-) longer than 10 bp.
- 4 From file cut_awk_test_file.tsv remove with sed column Description
 ("Assembly of # reads: ...").
- 6 Think about any task (manipulation with your data, ...) you are (sometimes) dealing with, which could be simplified/solved by using regular expressions. Try to solve it. Discuss it with others.

Basic skeleton	BASH	variables	Functions	Reading variables	В	ranching the code	1	Loops	

Scripting Basics of writing scripts in BASH

Scripting

 Basic skeleton
 BASH variables
 Functions
 Reading variables
 Branching the code
 Loops

Keeping correct syntax might be sometimes tricky. Use some checker helping you to fix your code, e.g. ShellCheck (on-line or locally shellcheck myscript.sh).

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Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	L	.oops	

Basic script

- Every script begins with **#!/bin/bash** (or alternative for another shells, Perl, ...)
- Add any commands you like...
- Every script should end with **exit** (but it is not necessary)
- After writing the script, add execution permission
 (chmod +x noninteractive.sh), launch with ./noninteractive.sh
- The most simple script:

```
#!/bin/bash
# Simple non-interactive script - no communication with user,
# only list of commands - prints user name, date, $PATH and free space
echo "Hi, ${USER}, today is $(date) and your PATH is ${PATH}."
echo "Free space on your disk:"
df -h
echo
exit
```

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	l	Loops	

Special BASH internal variables available in the script (selection)

- These variables can be used within script e.g. to parse arguments provided by the user
- \$1, ... (number from 1 up to number of parameters) individual positional parameters (see further examples)
- **\$0** path of the starting script
- **\$#** number of command-line arguments
- $\* all of the positional parameters, seen as a single word, must be quoted (i.e. " $\* ")
- \$@ same as \$*, but each parameter is a quoted string the parameters are passed intact, without interpretation or expansion, each parameter in the argument list is seen as a separate word, should be quoted (i.e. something like "\$@")
- \$\$ process ID (PID) of the script itself
- \$? Exit status of previous command, function, or the script itself
- See more variables...

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Basic skeleton	BASH	variables	Functions	Reading variables	1	Branching the code	Loops	

Functions in BASH

Pieces of code, which can be used repeatedly

```
# Declare new function within script
<sup>2</sup> function MyNewFunction1 {
   echo "Hello, ${USER} from $(groups) on ${HOSTNAME}!"
5 # Use it in a script as any other command
6 . . .
7 MyNewFunction1
8 . . .
• # Use with variables - provide parameters for the function
<sup>10</sup> # See following script examples for another input - same as in scripts
function MyNewFunction2 {
echo "The sum is $(("$1" + "$2"))."
13
<sup>14</sup> # Use it in the script as any other command
<sup>15</sup> MyNewFunction2 5 8 # For example
16 . . .
                                                                            r = r = -\tau \propto 0
```

Introduction								
Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	l	_oops	

It is important to check user input...



https://xkcd.com/327/

- By accident or purpose (attack), user can enter unexpected value
 - In the "best" case, the script "just" crashes
 - Script can behave unexpectedly, returning very weird results, damage data
 - Internal functions/commands can return error messages, which are hard to understand
 - Attacker can e.g. modify web content (XSS, ...), obtain private data, root privileges, ...
 - Applies also to scientific data wrong input use to have unexpected outcomes...
- Programmer should always check if user input is correct, filter it

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	L	.oops	

Script reading two variables

#!/bin/bash

```
2 # Arguments are read from command line as parameters of the script
3 # Order has to be kept (well, not in this case, but generally yes)
4 echo "Sum of two numbers $1 and $2 is $(("$1" + "$2"))." # $((calc...))
5 # "$#" is available every time and contains number of parameters
6 # (variables) given to the script
7 echo "Number of parameters is: $#"
8 # "$*" is available every time and contains all supplied parameters
9 echo "Those parameters were supplied: $*"
10 # "$0" is available every time and contains script path
11 echo "Path to the scrip is: \"$0\""
12 exit
```

When done, do:

- chmod +x interactive1.sh
- 2 ./interactive1.sh 8 9 # Or select any other two numbers
 - There is no checking of input values, nothing advanced, ...

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Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	1	Loops	

Variables will be interactively provided by the user

```
#!/bin/bash
```

2 # Arguments are read from user input (script asks for them)

 $_{3}$ echo "Please, input first value to sum and press 'Enter'"

```
4 read -r V1
```

5 echo "Please, input second value to sum and press 'Enter'"

```
6 read -r V2
```

```
_{7} echo "Sum of two numbers \{V1\} and \{V2\} is (("V1" + "V2"))."
```

```
8 # Note above that "$" is unnecessary on arithmetic variables
```

```
9 echo
```

```
10 exit
```

When done, do:

```
chmod +x interactive2.sh
```

- 2 ./interactive2.sh # Values will be provided when script asks
 - There is no checking of input values, nothing advanced, ...
 - See next slide to read the variable in while cycles to ensure it is correctly entered

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	Loops	

Ensuring user interactively provides correct input (while)

- Detailed explanations of all features used here are in various following slides... See scripts interactive2 {whiles, functions}.sh
- 1 ... # Following code replace lines 3 and 4 from previous script
 2 NUMBER='^[0-9]+\$'
- 3 echo "Please, provide a number as input value:"
- 4 while : # Start of while cycles run until correct input is provided
 - do # Star of the body of the cycles
- ⁶ read -r INPUT # Here the input from keyboard is received
- 7 if [[\${INPUT} =~ \${NUMBER}]]; then # Test if INPUT is a number 8 echo "OK, input value is \$INPUT."
 - break # We have correct value, we can break the cycles and continue
 - else # What to do if the user did not provided correct value
 - echo "Error! You provided wrong value!" # Tell the user
 - echo "Try again (the number):" # Ask user for new input value
- 13 **fi** # End of the conditional evaluation
- done # End of the while cycles
- $_{\scriptscriptstyle 15}$... # The code continues... Such check is needed for every variable...

9

10

11

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	1	Loops	

Ensuring user interactively provides correct input (function) I

```
# Regular expression to check if the provided input is a~number
_{2} NUMBER='^[0-9]+$' # From beginning (^) to end ($) only numbers
   Function to read and check user input (this goes to beginning)
3 #
4 function checkinput {
   while :
5
      do # Star of the body of the cycles
        read -r INPUT # Here the input from keyboard is received
7
        if [[ ${INPUT} =~ ${NUMBER} ]]; then # Test if $INPUT is a number
8
          echo "OK, input value is ${INPUT}."
9
          break # We have correct value, we can break and continue
10
          else # What to do if the user did not provide correct value
            echo "Error! You provided wrong value!" # Tell the user
12
            echo "Try again (the number):" # Ask user for new input value
13
           fi # End of the conditional evaluation
14
      done # End of the while cycles
15
      # Read variable is in INPUT
16
```

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	L	.oops	

Ensuring user interactively provides correct input (function) II

```
# Replace line 4 of interactive2.sh by (similarly for line 6)
...
checkinput # Use function declared on previous slide
V1="${INPUT}"
...
checkinput # Recycle the function to read next variable
V2="${INPUT}"
...
```

- User can provide as arguments...
 - Input/output data file names
 - Parameters for running whatever analysis can be passed to some scientific software within script or so
 - Which branch of the code to run

```
• ...
```

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Basic skeleton	BASH	variables	Functions	Reading variables	В	ranching the code	1	Loops	

Provide named parameters

```
#!/bin/bash
<sup>2</sup> # Script has only one parameter ($1) provided
# "case" is evaluating provided parameter and behaving accordingly
₄ case "$1" in
    d disk) # "|" means alternatives - more possible inputs
      echo "Your disk usage is:"
6
   df -h::
7
    u uptime)
8
      echo "Your computer is running:"
9
      uptime
10
    # This should be every time last possibility - any other input
11
    # User is then notified he entered nonsense and gets some help
12
    *) # Anv other input
13
      echo "Wrong option! "
14
      echo "Usage: 'd' or 'disk' for available disk space or 'u' or"
15
      echo " 'uptime' for computer uptime"
16
# Ends on next slide...
```

Basic skeleton	BASH	variables	Functions	Reading variables	В	ranching the code	Loops	

Notes to previous script

```
# ...end from previous slide
exit 1;; # In this case, exit with error code 1
esac
exit
```

- First make interactive3.sh executable and launch it via e.g. ./interactive3.sh d or ./interactive3.sh uptime or so
- Function **Case** has basic checking of input available as last parameter use *) any other input except those defined above will produce some warning message, error or so
- In same way can be added more parameters (by multiple use of <u>case</u> or by wrapping <u>case</u> by <u>while</u> loop), in the latter variant order of parameters does not have to be kept and all parameters are compulsory
- **Case** can evaluate simple regular expressions, e.g. **[Uu]ptime**, **d***, ...
- This is the most simple usage, more complex possibilities are ahead

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	1	Loops	

Provide parameters, verify them and behave accordingly I

```
#!/bin/bash
_{2} # From the beginning (^) to the end ($) at least one (+) number ([0-9])
_{3} NUMBER= ' ^ [ 0 - 9 ] + $ '
4 function usagehelp { # Function to print help - we will use it four times
    echo "Usage: number1 plus/minus/product/quotient number2"
5
    echo "Use plus for sum, minus for difference, product"
6
   echo " for multiplication or quotient for quotient."
7
8 exit 1 # End up with an error
0
if [[ "$#" -ne "3" ]]; then # Do we have 3 parameters provided?
    echo "Error! Requiring 3 parameters! Received $# ($*)."
11
    usagehelp # The function to print help
12
   fi # "=~" means testing if $1 fits to regular expression in $NUMBER
13
if [[ ! $1 = ~ ${NUMBER}]]; then # Is parameter 1 number?
   echo "Parameter 1 is not an integer!"
15
16 # Continues on next slide...
```

 Introduction
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 Basic skeleton
 BASH variables
 Functions
 Reading variables
 Branching the code
 Loops

Provide parameters, verify them and behave accordingly II

```
# Remaining part from previous slide...
    usagehelp # The function to print help
_4 if [[ ! 3 = ~  {NUMBER} ]]; then # Is parameter 3 number?
    echo "Parameter 3 is not an integer!"
    usagehelp # The function to print help
    fi
8 case "$2" in
    plus) echo "$(($1 + $3))";;
9
    minus) echo "$(($1 - $3))"::
10
    product) echo "$(($1 * $3))";;
11
    quotient) echo "$(($1 / $3))";;
12
    *) echo "Wrong option!"
13
      usagehelp # The function to print help
14
15
16
17 exit
```

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	L	.oops	

Provide parameters, verify them and behave accordingly III

```
# Make in executable and run it...
```

```
2 chmod +x interactive4.sh
```

```
3 ./interactive4.sh 7 plus 5 # For example...
```

- Note that we can evaluate input parameters in any order
- Compare syntax styling of **case** on previous slide and in script file interactive4.sh
 - Each option can be on single line, or on multiple lines
 - For each **case** option there can be any number of commands
 - There can be any number of **case** options convenient way how to evaluate multiple options in single step
 - Se following slides for most common usage of case
- **case** can be used anywhere in the code, not only to evaluate input parameters (as possible alternative to **if-else** branching)

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Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	L	.oops	

Multiple switches in classical UNIX form (no positional) I

- Following code use to be near beginning of the script to evaluate input
- See interactive5.sh for complete example
- getopts reads short (one-letter) parameters, they can have input value (marked by :)

```
#!/bin/bash
<sup>2</sup> # All provided values are evaluated in while cycles...
while getopts "hvi:o:a:" INITARGS do # Switches are -h -v -i -o -a
    case "${INITARGS}" in # $INITARGS contains the parameters to evaluate
      h|v) # Accept parameters "-h" or "-v" for help
        echo "Usage options..."
6
        exit # Terminate after providing help
7
      # End of this option
8
     i) # Parameter "-i" accepts some value (e.g. "-i inputfile.txt")
9
        ... # Do some checking etc...
10
        INPUTFILE="${OPTARG}" # $OPTARG always contains value of parameter
11
     # End of this option
12
# ...continues on following slide...
```

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	l	_oops	

Multiple switches in classical UNIX form (no positional) II

```
1 #
    ... starts on previous slide...
      o) # Parameter "-o" accepts some value (e.g. "-o outputfile.txt")
2
        ... # Do some checking etc...
3
        OUTPUTFILE="${OPTARG}" # $OPTARG always contains value of parameter
4
        # End of this option
5
      a) # Parameter "-a" accepts some value (e.g. "-a X" for number)
6
        # Check if provided value makes sense (integer between 10 and 300)
7
        if [[ "${OPTARG}" =~ ^[0-9]+$ ]] && [[ "${OPTARG}" -ge 10 ]] &&
8
          [[ "${OPTARG}" -le 300 ]]; then # The condition is long...
9
          VALUE=${OPTARG} # $OPTARG always contains value of parameter
10
          echo "Value is OK: ${VALUE}"
11
          else.
12
           echo "Error! For parameter \"-a \" vou did not provide an"
13
           echo " integer ranging from 10 to 300!"
14
           exit 1
15
          fi
16
17 # ...continues on following slide...
```

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	1	Loops	

Multiple switches in classical UNIX form (no positional) III

```
... continuing from previous slide...
      # End of this option (see previous slide)
2
      ?)
        echo "Invalid option(s)!"
4
        echo "See \"\$0 -h\" for usage options."
5
     exit 1
6
    # End of this option
7
8
    done # ... the end.
0
   Check if all required values are provided
10 #
" if [[ -z "${INPUTFILE}" ]] || [[ -z "${OUTPUTFILE}" ]]; then
    echo "Error! Name of input and/or output file was not provided!"
12
    echo "See \"\$0 -h\" for help usage..."
13
    exit 1
14
   fi
15
<sup>16</sup> # ...ends on following slide...
                                                           ・ロット 中国 マイヨット ヨー うらつ
```

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	Loops	

Multiple switches in classical UNIX form (no positional) IV

```
# ...continuing from previous slide...
<sup>2</sup> if [[ -z "${VALUE}" ]]; then
_{3} echo "Warning! Value for \"-a\" was not provided! Using default (10)."
_4 VALUE=10
5 fi
6 # Do the job...
7 for (( I=1: I<="${VALUE}": I++ )); do # Repeat task number of times</pre>
   echo -ne "Cycle {I}...\r" # Write number of cycle and return cursor to
8
         # the beginning of the line to overwrite the number in next step
9
    sleep 1s # Wait 1 second - just for fun ;-)
10
   # Do the task - append input to the output - note usage of variables
11
   cat "${INPUTFILE}" >> "${OUTPUTFILE}" #Do the job: append input to output
12
13
_{14} echo -ne "\n" # Reset cursor to new line
15 echo "Done!"
16 exit
```

Introduction Linux UN*X Command line Text Scripting Software MetaCentrum Git Administration The End Basic skeleton BASH variables Functions Reading variables Branching the code Loops

Multiple switches in classical UNIX form (no positional) V

- Script interactive5.sh contains complete example
- This is the classical way how to use UNIX switches used in most of commands
- while loop encapsulating **Case** ensures we evaluate all provided parameters regardless their number or order
 - Be prepared that user can use the arguments in any combination and order (e.g. calling -h together with any other switch) avoid in code doing several things at once

```
# Make it executable
chmod +x interactive5.sh
# Start with displaying help
./interactive5.sh -h # Or ./interactive5.sh -v
# Try it as common command line tool
./interactive5.sh -i input.txt -o output.txt -a 50
# Order of parameters doesn't matter
./interactive5.sh -o out.txt -a 50 -i input.txt
```

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Basic skeleton	BASH	variables	Functions	Reading variables	E	Branching the code	l	Loops	

```
Simple providing of input file I
```

Probably the most common script type you need - just specify data to process

```
#!/bin/bash
<sup>2</sup> # We expect exactly one parameter
3 if [[ "$#" -ne "1" ]]: then
4 echo "Error! Exactly one parameter is required!"
s exit 1
6 fi
7 # Verify that file exists and is readable
8 if [[ ! -r "$1" ]]: then
echo "Error! The file provided does not exist or is not readable!"
   exit 1
10
   fi
11
<sup>12</sup> # Do the operation with input file..
echo "Size of the file is $(du -sh "$1" | cut -f 1)."
_{14} echo "The file has (wc -1) = (ut -d) - (ut -f) lines."
15 echo "Making backup of the file $1..."
<sup>16</sup> # Ends on next slide...
```

```
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        Basic skeleton
        BASH variables
        Functions
        Reading variables
        Branching the code
        Loops
```

Simple providing of input file II

```
# ...the end from previous slide
# Copy file to backup (*.bak). If it succeeds, report it, if it fails
# exit with error (still handling single variable $1)
{ { cp "$1" "$1".bak && echo "Backup saved as $1".bak; } || \
        { echo "Error! Making backup of $1 failed!"; exit 1; }
        echo "Done!"
        exit
```

- Common way for simple scripts check input and do something with single input file
- Note lines 4 and 5 above common way to report success as well as handle failure
- Possibly add extra variables describing what to do with input data (e.g. slide 272)

```
# Make it executable
```

- 2 chmod +x interactive6.sh
- 3 # Use the script with some text file...
- 4 ./interactive6.sh long_text.txt

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Introduction								
Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	1	Loops	

If branching (examples are elsewhere)

```
# Basic variant - commands are done only if condition is met
<sup>2</sup> if condition: then
      commands
s if condition: then # Two branches - when condition is met and when not
      commands1 # condition is TRUE
   else
      commands2 # condition is FALSE - all other cases
   fi
<sup>10</sup> # Join together two (or more) if branches
if condition1: then
      commands1
12
    elif condition2: then
13
        commands2
14
  else
15
        commands3
16
      fi # Branching can be long, hard to read and susceptible to errors
17
```

Basic skeleton	BASH	variables	Functions	Reading variables	E	Branching the code	Loops	

Evaluation of conditions I

- Basic method to branch code do something according to certain condition
- Very versatile, usually there are more options how to write desired conditioning
- Avoid long chaining of conditions using **elif** statement (previous slide) susceptible to mistakes, hard to debug
- "[...] " (always keep space inside around it) is function to evaluate expressions
 - if ["\${VAR}" -eq 25] or alternatively test "\${VAR}" -eq 25 instead
 - if ["\${VAR}" == "value"]; ...
 - Escaping variables and values by double quotes ("...") is recommended (to be sure), but not strictly required all the time
 - if [! -f regularfile]; ... ! reverts condition
 - Single-bracket conditions file, string, or arithmetic conditions
 - Double-bracket syntax enhanced (now preferred)
 - Allow usage of regular expressions and globing patterns

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Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	Loops	

Evaluation of conditions II

- Word splitting is prevented **\${STRINGVAR}** can contain spaces etc.
- Expanding file names if [[-a *.sh]] (variant with only one bracket doesn't work when there are multiple sh files)
- More detailed test, e.g. if [[\$num -eq 3 && "\${STRINGVAR}" == XXX]]...
- Common tests
 - -eq Equal to (like ==)
 - -lt Less than
 - -gt Greater than
 - -ge Greater than or equal to
 - -le Less than or equal to
 - **-f** "**\$**{**FILE**}" True if **\$FILE** exists and is a regular file (not link or so)
 - -r "\${FILE}" True if **\$FILE** exists and is readable

Basic skeleton	BASH	variables	Functions	Reading variables	I	Branching the code	Loops	

Evaluation of conditions III

- -w "\${FILE}" True if **\$FILE** exists and is writable
- -x "\${FILE}" True if **\$FILE** exists and is executable
- -d "\${FILE}" True if **\$FILE** exists and is a directory
- -s "\${FILE}" True if **\$FILE** exists and has a size greater than zero
- -n "\${STR}" True if string \$STR is not a null (empty) string
- -z "\${STR}" True if string \$STR is a null string
- "\${STR1}" == "\${STR2}" True if both strings are equal
- "\${STR}" True if string \$STR is assigned a value and is not null
- "\${STR1}" != "\${STR2}" True if both strings are unequal
- -a Performs the AND function ([... -a ...] or [...] && [...])
- - o Performs the OR function ([... o ...] or [...] || [...])

4 = + 4 = + 9 < 0</pre>

Basic skeleton	BASH	variables	Functions	Reading variables	I	Branching the code	Loops	

Evaluation of conditions IV

- if statement can test whatever returning TRUE / FALSE, commonly something like if grep -q XXX; then ... (see also further)
- Do not confuse globing patterns and regular expressions when using [[...]]
 - Shell globing: if [["\${STRINGVAR}" == ?[sS]tring*]]; then ? represents single character [] any character inside and * zero or more characters
 - Regular expressions: if [["\${STRINGVAR}" =~ .[sS]tring.*]]... .
 represents single character (? would be zero or one occurrence of preceding expression), [] any character inside and .* zero or more occurrences of any single characters
 Same expression is interpreted in different ways

Introduction Linux UN*X Command line Text Scripting Software MetaCentrum Git Administration The End Basic skeleton BASH variables Functions Reading variables Branching the code Loops

Selecting version of RAxML according the CPU type I

- RAxML can take advantage of modern CPUs to highly speed up calculations, with or without parallelization — every version has separated binary, user must select, see README
- After compilation, the script can select e.g. on remote server appropriate version
- RAxML binaries must be in **\$PATH**
- See raxml_if.sh for whole script

```
if grep -iq avx2 /proc/cpuinfo; then # Does the CPU support AVX2?
RAXML='raxmlHPC-AVX2' # Select appropriate binary
elif grep -iq avx /proc/cpuinfo; then # Does the CPU support AVX?
RAXML='raxmlHPC-AVX' # Select appropriate binary
elif grep -iq sse3 /proc/cpuinfo; then # Does the CPU support SSE3?
RAXML='raxmlHPC-SSE3' # Select appropriate binary
else # The very last option
RAXML='raxmlHPC' # Slowest oldest CPU...
fi # End of branching
${RAXML} -s ${INPUT} # All the parameters as usually...
```

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	l	Loops	

Selecting version of RAxML according the CPU type II

Multiple branching in one step

- Same task as on previous slide, but instead of if-then branching it is using **Case**
- See raxml_case.sh for whole script

```
# Determine which CPU is available and which binary use then
<sup>2</sup> CPUFLAGS=$(grep -i flags /proc/cpuinfo | uniq)
a case "${CPUFLAGS}" in
    *avx2* |*AVX2*) # Does the CPU support AVX2?
      RAXML='raxmlHPC-AVX2';; # Select appropriate binary
    *avx* | *AVX*) # Does the CPU support AVX?
6
      RAXML='raxmlHPC-AVX';; # Select appropriate binary
7
    *sse3* | *SSE3*) # Does the CPU support SSE3?
8
      RAXML='raxmlHPC-SSE3':: # Select appropriate binary
9
    *) # The very last option
10
      RAXML='raxmlHPC':: # Slowest oldest CPU...
    esac # End of branching
12
<sup>13</sup> {RAXML} -s {{INPUT} # All the parameters as usually...
```

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	Loops	

For loops I

- for loops are available in practically every programming language
- BASH allows plenty of variants how to declare repetitions
- In for loop we know in advance number of repeats numerical sequence, list of files, ...
- Common way how to do same operation with multiple files

```
# Ways how to declare number of repetitions
# Ways how to declare number of repetitions
# Variable $I contains in every repeat number from 1 to 10 - number of
# respective repeat
for I in $(seq 1 10); do echo "${I}"; done # "seq" is outdated
for I in 1 2 3 4 5 6 7 8 9 10; do echo "${I}"; done
for I in {1..10}; do echo "${I}"; done
for (( I=1; I<=10; I++ )); do echo "${I}"; done
# One line for cycle for resizing of multiple images
# Variable $JPGF contains in every repeat one-by-one name of input file
# (each JPG) processed in the respective turn (creates tuhmbnails th-...)
for JPGF in *.jpg; do convert ${JPGF} -resize 100x100 th-${JPGF}; done
# Contains in the respective turn (creates tuhmbnails th-...)
# Contains the test of test of the test of test
```

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	I	Loops	

For loops II

• Basic way to process more files

```
# More commands in a block
<sup>2</sup> for JPGF in *.jpg do
    echo "Processing JPG file ${JPGF}"
   file "${JPGF}" # Get information about currently processed file
   # Create tuhmbnail. If it fails, skip following commands
5
    convert ${JPGF} -resize 100x100 thumbs-${JPGF} || continue
6
    echo "File thumbs-${JPGF} created"
7
8
。#
   Passing through each loop can be influenced using conditions and
    subsequent skipping of rest of the loop
10 #
for ...; do # Start cycles as you need
    commands1 # commands1 will be executed in any case
12
   if (condition): then # Set some condition to skip commands2
13
      continue: fi # Go to next iteration of the loop and skip commands2
14
   commands2
15
```

done

16

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	I	Loops	

While and until loops I

```
# while loop is evaluating condition and if it is equal to 0 (TRUE)
<sup>2</sup> # the loop body is launched, repeatedly while the condition is met
while condition: do
      commands
done
6 # Like while loop, but until condition is NOT equal to zero (not met)
<sup>7</sup> until condition: do
   commands
done
<sup>10</sup> # Compare differences between while (more common) and until loops
II I=0 # Assign initial value
<sup>12</sup> # Repeat while I is lower or equal 10; in every step increment I by 1
<sup>13</sup> while [ $I -le 10 ]; do echo "Value: $I"; I=$(($I + 1)); done
I_{14} I=20 # Assign initial value
_{15} # Repeat until I is lower then 10; in every step decrement I by 1
16 until [ $I -lt 10 ] do echo "Value: $I": I=$(($I - 1)) done
```

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Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	I	_oops	

While and until loops II

'continue' skips to another loop turn, 'break' terminates running ² # of whole loop (no further turns) and skips to following commands while ...; do # Start loops as you need commands... if [condition]; then # If something happens 5 break # End up the loops and continue by following commands ⁸ # While loops are popular to process every line of input file 9 # The text file use to contain e.g. list of files to process (if for ¹⁰ # whatever reason 'for' loop construction is impractical) while read TEXTLINE; do # Run loops on every line of text file commands... # TEXTLINE contains in each turn one line of the file 12 done < text_file_to_process.txt # Commonly list of input data files 13 14 # Infinite loops - common when waiting for some condition to proceed while : do echo "Press CTRL+C to exit..." done 16 for (()) do echo "Press CTRL+C to exit..." done

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Basic skeleton	BASH	variables	Functions	Reading variables	B	Branching the code	Loops	

What is worth of scripting

- Any task you need to repeat from time to time requiring more commands almost anything :-) Programmers are lazy. Do not manually do work worth of trained apes.
 - Take advantage of usage of loops, conditions, variables, ...
- Processing of multiple files
 - Various manipulations (conversions, ...)
 - Parsing (e.g. extracting information from multiple CSV or logs)
- Repeated running of some analysis (requiring multiple steps)
 - Keep settings and all preparing and post-processing steps
- Anything you do often and it requires non-trivial set of commands
- And much more...

Start scripting, coding

Now you should have enough knowledge to start writing scripts to do such tasks. Start with something simple, solving some your practical need (e.g. for MetaCentrum, from slide 262). You'll gather experience and improve.

Basic skeleton	BASH	variables	Functions	Reading variables	Branching the code	1	Loops	

Scripting tasks

- Write short script (or at least concept how it should work) to print file name of JPG file and its dimensions in px. Use e.g. file or ImageMagick identify to get the dimensions.
- 2 Write short script (or at least concept how it should work) taking as input arguments file name and taxon name, verify their validity, extract respective FASTA sequence and print it to standard output.
 - Work on file Oxalis_HybSeq_nrDNA_selection_alignment.fasta.
- Think about several tasks where you would use BASH scripts to automatize repeated work and/or processing of multiple files.
 - Think about usage of various loops (and/or GNU Parallel), if-then branching, various conditions, etc.
 - Prepare concept(s) of such script(s).

Keep in mind...

Do not do simple repeated work worth of trained monkey manually. It is silly. Every such task is worth of (one-line) script to work instead of you.

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Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Software

Software

Packages

Compilation

Java

Windows applications

Scientific applications

Games

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Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Package management I

Installation of software

- **Package** an application or its part (documentation, plug-ins, translations, ...)
- Packages are available in **repositories** (directories) on the internet
 - System has list of applications available
 - Updates and bug fixes are installed for all applications using one interface (GUI or command line) very reliable
 - Packages are digitally signed security
 - User can set custom repositories to get more package resources
 - Repositories can be added whenever needed check documentation for your distribution (at least basic "how-to")
- The most different task among Linux distributions
- Packages have dependencies required shared libraries and so on use package manager and try to avoid downloading packages from the internet outside repositories
- Read manual for your distribution!

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Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Package management II

Installation of software

- Package is basically an archive and system has configured directories where to unpack it binaries are commonly in /usr/bin/, shared libraries in /usr/lib and /usr/lib64, data in /var, ...
- User should not care where parts of packages go to system is taking the care user can only damage it
- Shared libraries are installed automatically whenever required
- As all files are placed in standard defined directories, it is very simple to use them also for another applications
- Applications not available in repositories, neither as distributional package should be installed into ~/bin for current user or /usr/local for all users (binaries then go into /usr/local/bin and so on)

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Packages	Compila	tion	Java	Windo	ows applications	Scientific applications	Games	

Package management III

Installation of software

- Common distributions use to provide convenient graphical tool to manage software
 - Ubuntu Software Center
 - Synaptic feature rich, graphical, advances, for any DEB distribution (Debian, Ubuntu, Mint, ...)
 - Aptitude feature rich, command-line, advanced, for any DEB distribution (more advanced version of Apt)
 - DPKG low-level, any DEB-based distribution
 - YaST Software for openSUSE (feature rich, graphical as well as command-line)
 - Zypper feature rich, command-line, advanced, for openSUSE
 - DNF feature rich, command-line, advanced, for Fedora and another RPM based distributions (replacing older Yum)
 - RPM low level, any RPM-based distribution
 - GNOME software in most of distributions using GNOME
 - And many more...

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Packages	Compila	tion	Java	Windo	ows applications	Scientific applications	Games	

Package management IV

Installation of software

- All do same task as soon as user master one, others are equally simple
- Distributions use to provide convenient update applet notifying about awaiting updates
- There use to be web services to look for packages, also from other sources openSUSE, Debian, Ubuntu (+ Launchpad and PPAs), Fedora, ...
- The task is always same, the exact work-flow and commands more or less differ among distributions...
- Tools like Android Google Play, Apple Store or Windows Store are inspired from Linux (but terribly simplified)...

Task

Install some new software into your Linux. Use graphical as well as command-line tools. See following slides for instructions.

Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Package management in command line in openSUSE and SLE (basic commands) I

- Root password is required: use sudo ... or su -
- Package name * . rpm
- zypper in package install package
- **zypper rm** *package* remove *package*
- zypper ref refresh repositories
- zypper up update
- zypper dup upgrade to newer release of whole distribution (see documentation)
- zypper ps -s check which running applications (including SystemD services) should be restarted after update of packages

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Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Package management in command line in openSUSE and SLE (basic commands) II

- zypper se *term* search *term*
- zypper pa --orphaned --unneeded list packages, which can be safely removed
- **yast sw_single** interactive manager
- zypper lr list repositories
- zypper ar *repository* add *repository* (URL of remote *. repo file)
- **zypper rr** *repository* remove *repository* (name according to **zypper lr**)
- zypper mr *repository* modify *repository* (see man zypper first, or use yast sw_single)

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Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Package management in command line in openSUSE and SLE (basic commands) III

- **zypper** pa **package** get information about particular **package** or another query (e.g. list of dependencies, see **man zypper**)
- **opi** *package* search (and possibly install) *package* in OBS in all repositories contributed by users (take care, there are no quality checks)
- rpmconfigcheck check which configuration files in /etc have new version after update of some software — compare respective configuration files with new *.rpmnew files
- **rpm**^{*} commands for other tasks
- man zypper, man rpm usage help

Packages	Compila	tion	Java	Windo	ows applications	Scientific applications	Games	

Package management in command line in Debian/Ubuntu and derivatives (basic commands) I

- Root password is required: use sudo ... or su -
- Package name * . deb
- apt install package install package
- apt remove package remove package
- apt update refresh repositories
- apt upgrade upgrade packages
- apt dist-upgrade upgrade to newer release of whole distribution
- apt search term search term
- apt autoremove clear unneeded packages

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Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Package management in command line in Debian/Ubuntu and derivatives (basic commands) II

- apt autoclean cleanup of files after uninstalled packages
- aptitude interactive manager
- cat /etc/apt/sources.list list repositories
- nano /etc/apt/sources.list add/remove/edit repositories
- dpkg-*
 , apt-*
 commands for other tasks
- aptitude is used in similar way as apt (e.g. aptitude install package, ...) or as interactive tool (just run aptitude)
- Similar tasks can be done with apt, apt-get, or aptitude

• man aptitude, man apt-XXX, man dpkg-XXX, man apt — usage help

Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Package management in command line in RedHat, Fedora, CENTOS and derivatives (basic commands) I

- Root password is required: use sudo ... or su -
- Package name * . rpm
- dnf install package install package
- dnf remove *package* remove *package*
- dnf check-update refresh repositories, check for updates
- dnf upgrade upgrade packages
- dnf search *term* search *term*
- dnf autoremove clear packages
- dnf info package get information about package

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Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Package management in command line in RedHat, Fedora, CENTOS and derivatives (basic commands) II

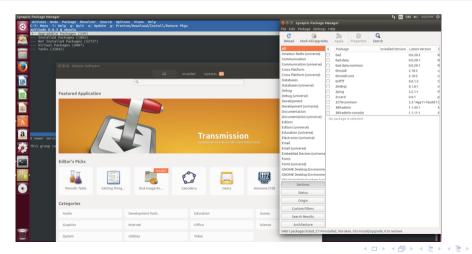
- dnf repolist list repositories
- dnf config-manager manage repositories and another settings
- rpm -Uvh package.rpm install locally downloaded package.rpm
- rpm -e package remove package
- rpm* commands for other tasks
- In older releases of Fedora, RedHat and CENTOS, yum is used instead of dnf in nearly identical way
- man dnf (or man yum), man rpm usage help

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Packages	Compilat	tion	Java	Windo	ws applications	Scientific applications	Games	

Graphical package managers I

Ubuntu Software, and Synaptic and text-based Aptitude for all DEB-based distributions



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Packages	Compila	tion	Java	Windo	ows applications	Scientific applications	Games	

Graphical package managers II

GNOME Software in Fedora and YaST in openSUSE

Activities 📋 Software 🕶		Tue	12:40	ĥ	· • • • ·	Q	Ya5T2		
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			Builder An IDE TOT GNOME	i n	al l	Name Boysteen NON-OSS SS Packman	Package Mes-Ib0L1 Mes-Ib0L59/2-2 Mes-Ib0L59/2-2 Mes-Ib0L69/2-2 Mes-Ib0L69/2 ModerManager ModerManager	Summary Installed (Availab) The GU/GLX ru. 11.2.2.166.1 Free impleme 11.2.2.166.1 Meas VA/PI L. 11.2.2.166.1 DBus interface 14.1.4.1 ELE 50.1.0.45.1	e)
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• Practically every common general distribution has some graphical tool... Explore it...

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Packages	Compila	tion	Java	Windo	ows applications	Scientific applications	Games	

Manuals for package management

- openSUSE and SUSE Linux Enterprise: https://doc.opensuse.org/documentation/leap/startup/html/ book-startup/part-reference-software.html and https://en.opensuse.org/Portal:Zypper
- Red Hat, Fedora, CENTOS, Scientific Linux and others: http://yum.baseurl.org/ and newer

https://docs.fedoraproject.org/en-US/quick-docs/dnf/

- Debian (and derivatives): https: //www.debian.org/doc/manuals/debian-reference/ch02.en.html and https://wiki.debian.org/PackageManagement
- Ubuntu (and derivatives):

https://help.ubuntu.com/stable/ubuntu-help/addremove.html
and https://help.ubuntu.com/community/AptGet/Howto

• And another distributions...

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Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Basics of compilation

- Some software is distributed only as source code (e.g. downloaded from GitHub) written in languages like C or C++ user has to *compile* it to get working binary executable
- Compilation creates binary specific for particular operating system and hardware platform - can be tuned for optimal performance
- Interpreted languages (Bash, Perl, Python etc.) don't have to be compiled (but it is possible)

 they need their interpreter to run, relative easily portable among hardware platforms and OS (similar to Java and its Virtual Machine)
- Applications requiring compilation usually have good instructions
- If you don't have to do it, don't do it. Solving problems can be complicated contact someone skilled or author of the application, consult ChatGPT...
- 4 make # Basic building command, sometimes only this is required 5 make install # Placing everything into correct placed, sometimes required

Introduction								
Packages	Compila	tion	Java	Windo	ows applications	Scientific applications	Games	

Install tools needed for compilation

- You need to install compilation tools for your distribution and programming languages you are going to use
- Commonly, extra dependencies are required to compile the application
 - Packages for compilation use to end with <u>-dev</u> or <u>-devel</u> (e.g. if the software requires package <u>zlib</u> to run, install also its developmental version <u>zlib-dev(el)</u> to be able to compile it)
 - All requirements should be listed in README and/or INSTALL documents of particular package user must install them manually...
- # openSUSE and SUSE Linux Enterprise
 2 zypper in -t pattern devel_basis devel_C_C++
 3 # Debian, Ubuntu and derivatives like Linux Mint and others
 4 apt install build-essential # Or "aptitude install build-essential"
 5 # Red Hat, CENTOS, Fedora and derivatives (2 options dnf or yum)
 6 dnf groupinstall "Development Tools" "C Development Tools and Libraries"
 7 yum groupinstall "Development Tools" "C Development Tools and Libraries"

Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Compilation of RAxML

- Available from https://github.com/stamatak/standard-RAxML
- Before compilation check README
- This example does not require to run make install, it does not have extra dependencies for compilation, it requires specifying of particular source file by make -f (there are multiple GCC files, not just one main)
- mkdir raxml # Create working directory
- ² cd raxml/ # Go there
- $_{3}$ # Get source code from GitHub (svn downloads only changed files)
- 4 svn co https://github.com/stamatak/standard-RAxML/tags/v8.2.12
- 5 cd v8.2.12/ # Go to newly created directory
- 6 ls # List files
- 7 rm -rf Windows* # No need of Windows version delete it
- 8 # Compile standard version (other versions are available for better CPU)
 9 make -f Makefile.gcc
- 10 rm *.o # Remove unneeded files (temporal for compilation)
- n ./raxmlHPC -h # Launch it see RAxML help

Packages	Compila	tion	Java	Windo	ows applications	Scientific applications	Games	

Compilation of SAMtools

- See https://www.htslib.org/download/
- Ensure packages **zlib** and **zlib-dev(el)** are installed required for running and compilation, see INSTALL and README

wget https://github.com/samtools/samtools/releases/download/1.10/ samtools-1.10.tar.bz2 # Download SAMtools a tar xjvf samtools-1.10.tar.bz2 # Unpack the archive d cd samtools-1.10/ # Go to the unpacked directory 5 ./configure --help # See various configuring options 6 ./configure # Configure settings for compilation (default settings) 7./configure --without-curses # Compile without neurses support 8 make # Compile the software - check if there is error # Ensure developmental files for zlib (and neurses) are available 10 sudo make install # Copy products into final location - default /usr/local u sudo make prefix=/where/to/install install # Install into custom location ¹² make prefix=/home/\$USER/bin install # Binary into /home/\$USER/bin/bin ¹³ make clean # Cleanup - final files are already in the destination

Packages	Compila	tion	Java	Windo	ows applications	Scientific applications	Games	

Launching Java applications

- Java is probably the most portable language working on any operating system the only condition is to install Java virtual machine (JVM)
- Linux usually use OpenJDK search for packages named *openjdk*
- Let's download e.g. FigTree from https://github.com/rambaut/figtree/releases
- # Go to directory where you downloaded it
- 2 cd directory/with/downloaded/figtree
- 3 # Decompress downloaded archive
- 4 tar zxvf FigTree_v1.4.4.tgz
- 5 # Go to created directory
- 6 cd FigTree_v1.4.4/
- 7 ls * # List files, also in subdirectories
- 8 # Launch it (command java launches *.jar files)
- 🤋 java -jar lib/figtree.jar
- 10 # Limit its memory usage to 128 MB
- n java -Xmx128m -jar lib/figtree.jar

Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Windows applications on Linux I

- Applications written for one operating system do not work on the other systems...
 - They must be written in portable language like Java or script like Perl, Python or BASH
 - Otherwise we need an emulator not everything works
- Windows has since v. 10 possibility to run Linux applications, other option (for more Windows versions) is Cygwin (application must be specially compiled to work on Cygwin)
- To run Windows applications on Linux use Wine
 - Search for packages named wine and install it
 - Sometimes, extra functionality is in extra packages check wine-*
- To run DOS application on Linux use dosbox (package dosbox)
- As soon as Wine is installed, just click to Windows * . exe file...
- Windows applications are installed into ~/.wine/ where Windows directory structure is created, launchers use to be placed to standard application menu into **Wine** section

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Packages	Compila	tion	Java	Windo	ws applications	Scientific applications	Games	

Windows applications on Linux II

- Use winecfg to change settings (e.g. version of Windows can be different for each application, custom DLL library, ...)
- winefile starts Windows file browser, notepad Notepad, winemine Mines
- To install some extra parts required by some applications use winetricks
 - Usage use to differ according to distribution and GUI
 - Browsing and selecting items to install can be bit messy...
 - It can be hard to check application requirements if it fails, check if it is listed at https://appdb.winehq.org/ and/or run it from command line like wine application.exe and inspect errors in output
- Before installing Windows application under Wine, check if there is some native Linux application to fit your needs...
 - Plenty of applications are available for more operating systems
 - Linux distributions use to have external contributor's sites to provide more packages
 - For many Windows-only applications there are fully comparable alternatives

Introduction								
Packages	Compila	tion	Java	Windo	ows applications	Scientific applications	Games	

Windows applications on Linux III

- Some applications do not work under Wine (from various reasons), some complex packages are supported commercially (I have no experience with it)
- Wine is well compatible with rest of the Linux hosting system, but it is also considerable to install Windows in e.g. VirtualBox (or another virtualization platform), if needed



winefile, winetricks and winecfg

Introduction								
Packages	Compila	tion	Java	Windo	ows applications	Scientific applications	Games	

Where to get scientific applications for Linux I

- There is no universal simple solution
- As first step look if particular package is available for your distribution
 - Debian Science https://wiki.debian.org/DebianScience same packages are available also for Ubuntu, Mint and all the DEB derivatives
 - openSUSE Science project https://en.opensuse.org/Portal:Science
 - Fedora scientific packages https://fedoraproject.org/wiki/Scientific_Packages_List
 - Major distributions have web services (e.g. Launchpad for Ubuntu or openSUSE Build Service) where users can create their own personal repositories and package their favorite packages (like myself) search...
- There are projects creating repositories with custom management system providing (among others) plenty of scientific applications
 - Probably most known is Conda
 - Homebrew on Linux is derived from macOS Homebrew (works also on WSL) Brewsci with scientific packages, e.g. bioinformatics

Packages	Compila	tion	Java	Windo	ows applications	Scientific applications	Games	

Where to get scientific applications for Linux II

- Authors sometimes provide on homepages RPM/DEB/precompiled Java binaries/... check them first
- If there is no other option, download source code and compile yourselves...
 - Always check documentation for requirements and instructions
 - Solving issues requires experience, can be tricky, ask for help and don't give it up
- Scientific programming languages like R, Python, Perl, Julia, Matlab etc. have their own system to install language-specific packages
 - Distributions sometimes provide packages at least for part of the packages of such languages

 typically at least for Python, Perl or R this is especially convenient for packages having
 plenty of complex dependencies
- Packages in various repositories are sometimes not up-to-date with newest version released

 if so, contact maintainer of distributional package and kindly ask for update
 (distributional webs use to have easy ways how to do it)

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Introduction								
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How to game on Linux

- Plenty of games are in repositories of all major Linux distributions just search
- Many open-source games are multiplatform
- Some distributions have extra repositories for games, e.g. openSUSE
- See https://www.gamingonlinux.com/ for news etc.
- A lot of Windows-only games can be used with Wine
- Install Steam (package is often available in standard repositories) and there activate Proton (version of Wine to run plenty of Windows games on Linux via Steam)
- Although not all games available for Windows are available for Linux, there are more games than you have time... ;-)

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Information	Usa	age	Tasks		Graphical con	nection	More s	ervices	

MetaCentrum

MetaCentrum

 Information
 Usage
 Tasks
 Graphical connection
 More services

Vojtěch Zeisek (https://trapa.cz/)	Linux, command line & MetaCentrum	January 14 to 16, 2025	261/317

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Information	Usa	age	Tasks		Graphical conr	nection	More s	ervices	

CESNET and MetaCentrum I

- CESNET (česky) is organization of Czech universities, Academy of Science and other organizations taking care about Czech backbone Internet, one of world leading institutions of this type
- CESNET provides various services (česky)
 - Massive computations MetaCentrum (česky)
 - Large data storage (česky)
 - FileSender (česky) to be able to send up to 1.9 TB file
 - Cloud (česky) computing (HPC) cloud similar to e.g. Amazon Elastic Compute Cloud (EC2), Google Compute Engine or Microsoft Azure
 - ownCloud (česky) to backup and/or sync data across devices (default capacity is 100 GB, user may ask for more) similar to e.g. Dropbox, Google Drive or Microsoft OneDrive
 - It is possible to connect by webDAV to ownCloud (slide 139) many applications support it
 - It is possible to share calendars and/or address books via calDav and cardDav among devices and/or people
- Services accessible without registration

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Information	Usa	age	Tasks		Graphical con	nection	More s	services	

CESNET and MetaCentrum II

- ownCloud https://owncloud.cesnet.cz/
- FileSender https://filesender.cesnet.cz/
- · Go to web and log in with your institutional password
- Services requiring registration (and approval)
 - To use MetaCentrum fill registration form https://metavo.metacentrum.cz/en/application/form(česky)
 - To use data storage fill registration form https://einfra.cesnet.cz/perun-registrar-fed/?vo=storage
 - After registration for MetaCentrum, user can join MetaCloud via https://perun. metacentrum.cz/fed/registrar/?vo=meta&group=metacloud
 - Login is using EdulD (česky)
- Information about data storage https://du.cesnet.cz/en/start (česky) contains detailed usage instructions

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Information	Usa	ige	Tasks		Graphical con	nection	More s	services	

CESNET and MetaCentrum III

- Information about MetaCentrum https://www.metacentrum.cz/en/(česky) and documentation https://docs.metacentrum.cz/
 - The documentation is being migrated from wiki https://wiki.metacentrum.cz/wiki/Main_Page(česky)
- Information about MetaCloud https://docs.cloud.muni.cz/ (old wiki page)
- Also available is Galaxy https://usegalaxy.cz/ (same login as to MetaCentrum) — web based bioinformatics framework (more information at documentation)
- Current state and usage of resources is available at https://metavo.metacentrum.cz/en/(česky)
- Manage your user account at http://metavo.metacentrum.cz/en/myaccount/(česky)
- Personal view on actual resources and running tasks is at https://metavo.metacentrum.cz/pbsmon2/person

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Introduction									
Information	Usa	age	Tasks		Graphical con	nection	More :	services	

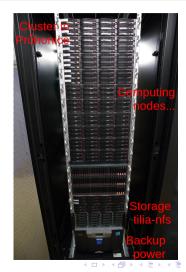
CESNET and MetaCentrum IV

- List of available applications https://docs.metacentrum.cz/software/
- MetaCentrum has 11 frontends where users log and thousands of computers doing the calculations they are not accessed directly to run task
- Most of computers are running Debian GNU/Linux
 - Basic usage as with any other Linux server SSH & command line...
 - Tasks are mainly submitted via scripts (see following slides)

Introduction									
Information	Us	age	Tasks		Graphical con	nection	More s	services	

Terminology

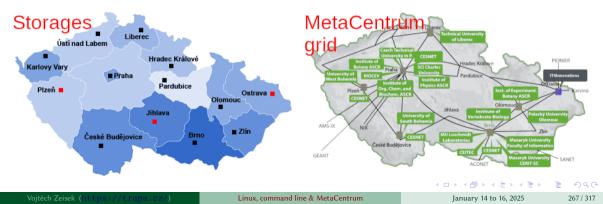
- Node (computing server) single computer, worker finally doing your computational job
- Cluster bunch of nodes in rack (special case storing nodes, use to contain also network switch, backup power, ... e.g. cluster in Průhonice, česky)
- Grid clusters distributed in various places, connected into single system by fast network (e.g. MetaCentrum, česky)
- Supercomputer extra powerful computer, nowadays mostly special cluster, e.g. IT4Innovations in Ostrava



Information	Usa	ige	Tasks		Graphical con	nection	More :	services	

Distributed topology I

- MetaCentrum clusters are distributed in various Czech cities (and institutions)
- Clusters use to have (at least small) storage array (accessible via /storage/...)
- There are special archive storages (česky) in Jihlava, Ostrava and Plzeň



Information	Usa	age	Tasks		Graphical conr	nection	More s	services	

Distributed topology II

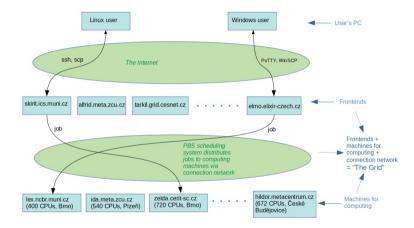
- Users have different quota on different arrays (depending on home organization etc.)
- There are 11 frontends where user logs via SSH and prepare computing task for submission etc. (see further)
- Distributed topology might be bit confusing user has different home directory when logging to different frontends recommended is to use as few frontends and storages as possible
- Some special services (like OnDemand) start on particular storage (here brno3)
- Generally, computing task loads data from selected storage and can start on any cluster
- Orientation is plenty of storages might be sometimes tricky ensure where you are and where your data are supposed to be
 - Preferably use single frontend and storage to avoid confusions and issues with paths

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Introduction L								
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Basic workflow



From old beginners guide

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MetaCentrum usage

- Transfer data into one of storages by e.g. scp from command line, WinSCP from Windows or FileZilla from any OS
- 2 Connect via SSH to selected frontend. Same credentials are used for all frontends, for SSH login as well as file transmissions
- 3 In home directory on the storage (accessed via frontend) prepare all needed data and non-interactive script to do the calculations
- Submit job using qsub. Tasks are not launched immediately, but submitted into queue and system decides when it will be launched
- **6** Monitor job progress. Check results. Etc...
- # Login to selected server (tarkil is located in Prague)
- ² ssh USER@tarkil.metacentrum.cz
- $_3$ # Continue as in any other command line...
- 4 qsub ... # Submit the job (see later)

Information	Usa	age	Tasks		Graphical con	nection	More :	services	

File transfers to MetaCentrum

- Graphical applications: e.g. FileZilla or most of Linux file managers
- Protocol is SSH/SSH2/SFTP/SCP, port 22, server is selected storage address — if possible, select any and keep using it
- All servers (storages, frontends, computing nodes) are accessible under domain *.metacentrum.cz – e.g. tarkil.grid.cesnet.cz is same as tarkil.metacentrum.cz
- See slide 139 and following to command-line transfers of files

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VirtualBox SloBca 16.1.2021.13		filesender	Složka 5.10.2
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aspera Složka 1.6.202113.4		gnupg	Složka 25.2.2
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bogofiter Složka 30.12.2016.2		java	Složka 27.1.2
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Information	Usa	age	Tasks		Graphical con	nection	More :	services	

Basic skeleton of script running tasks I

#!/bin/bash

² # Modify the script according to your needs!

3 # Set data directories

4 WORKDIR="my_data_dir" # Or something else

5 DATADIR="/storage/XXX/home/\${LOGNAME}" # Or other storage

6 # There is e.g. directory /storage/praha1/home/gunnera/my_data_dir

7 # containing all the data needed for calculations

8 # Clean-up of SCRATCH (it is temporal directory created by server) - the 9 # commands will be launched on the end when the job is done

10 trap 'clean_scratch' TERM EXIT

n trap 'cp -a "\${SCRATCHDIR}" "\${DATADIR}"/ && clean_scratch' TERM

12 # Change working directory - script goes to the directory where

¹³ # calculations are done

14 cd "\${SCRATCHDIR}"/ || exit 1 # If it fails, exit script

 $_{\rm 15}$ # Prepare the task - copy all needed files from working directory into

16 # particular computer which will finally do the calculations

¹⁷ # Ends on following slide...

Information	Usa	ige	Tasks		Graphical con	nection	More :	services	

Basic skeleton of script running tasks II

- # ... begins on previous slide; copy data if it fails, exit ² cp -a "\${DATADIR}"/"\${WORKDIR}"/* "\${SCRATCHDIR}"/ || exit 1 ³ # Prepare calculations - load required application modules 4 # See https://docs.metacentrum.cz/software/ 5 # Every application module is loaded by "module add XXX" 6 module add parallel/20210922-gcc-10.2.1-iiyjqem # In this (example) case 7 module add mrbaves/3.2.7a # GNU Parallel and MrBaves ⁸ # Launch the analysis - calculate MrBayes for multiple files 9 # Note Parallel will distribute task among 8 CPU threads (-j 8), so that ¹⁰ # gsub must in this case contain select=1:ncpus=8 (see further) in find . -name "*.nexus" -print | parallel -j 8 'mb {} | tee {.}.log' ¹² # Copy results back to \$DATADIR directory ¹³ cp -a "\${SCRATCHDIR}" "\${DATADIR}"/ || export CLEAN SCRATCH='false' ¹⁴ # This is all needed, the script is ready to be launched... 15 exit
 - Make metacentrum. sh executable and modify it to fit your needs...

Information	Usa	ige	Tasks		Graphical con	nection	More s	services	

Launching of tasks

- See https://docs.metacentrum.cz/computing/run-basic-job/
- Personal view https://metavo.metacentrum.cz/pbsmon2/person has nice overview of available resources and tasks and allows comfortable construction of submission command
- # We will run up to 5 days (120 hours), require one physical computer # with 8 CPU threads, 24 GB of RAM, 10 GB of disk space and we get all # information mails (for abort, beginning, exit) qsub -1 walltime=120:0:0 -1 select=1:ncpus=8:mem=24gb:scratch_local=10gb \ - m abe metacentrum.sh # Check how the task is running (above web) and qstat -u \$USER # Information about \$USER's jobs (queued and running) gstat 123456789 # The task ID is available from commands above or mail qstat -f 123456789 # Print a lot of details qdel 123456789 # Terminate scheduled or running task qextend 123456789.meta-pbs.metacentrum.cz 12:0:0 # Prolong walltime (12 h)

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Information	Usa	age	Tasks		Graphical con	nection	More s	services	

Key MetaCentrum commands

- MetaCentrum is "just" normal Linux server work there as on any other Linux system
- Command module loads/unloads selected application
- Tasks (BASH scripts) are submitted for computing by qsub the script must copy the data into \$SCRATCHDIR and do all calculations there
 - It has plenty of options how to specify requirements (see next slide and help)
- Queued and running jobs can be seen by **qstat** -u **\$USER** (**qstat** has much more options) and any job can be terminated by **qdel** 123456789 (number from **qstat**)

module add <TAB><TAB> # Load some module
module rm XXX # Unload selected module
module list # List of currently loaded modules
qsub ... # Submit task for computing - select any parameters needed
qstat -u \$USER # See \$USER's running and queued jobs
qdel 123456789 # Termite task (number from qstat)

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Scheduling details I

- Specify needed time
 - Always hours:minutes:seconds, so e.g. for 4 weeks use
 - -1 walltime=672:0:0 (28 · 24), for two days and 12 hours
 - -1 walltime=60:0:0
 - User may extend it with **qextend** (see **qextend info**), otherwise ask support (write them in advance)
- Ask for as much RAM as you need (e.g. -1 mem=8gb to request 8 GB)
 - If the task is going to require more, than allowed, system kills it...
 - If user doesn't use all required RAM, the system temporarily lowers priority for future tasks (RAM is limiting resource, do not waste it)
 - It can be hard to estimate (no easy general advice to estimate needs for particular task) do some experiment and see how your application behaves with your data...
- Disk space is relatively free resource, user can ask more to have some reserve (e.g.
 - -1 scratch_local=10gb to request 10 GB)

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Scheduling details II

- Specify how many physical computer(s) you are going to use (e.g. -1 select=1 for one machine) and number of CPU threads on each machine (e.g.
 - -1 select=1:ncpus=8 for 1 machine with 8 cores or
 - -1 select=2:ncpus=4 for 2 machines, each with 4 CPU threads)
 - It use to be necessary to specify correct number of threads for the application (e.g. parallel -j 4) the application sees all CPUs on the machine, but can't use them
 - If the application consumes less than required, the system temporarily lowers priority for future tasks, if it try to use more, it will be very slowed down or killed by the server
 - If using more physical machines, ensure correct settings of e.g. MPI (see documentation for respective software you are using)
- If requesting e-mails (e.g. -m abe to get mail about abort, beginning and exit of the task) and submitting plenty of tasks by some script, it can result in plenty of mails...

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Scheduling details III

- Every user has certain priority increased by acknowledgments (it's mandatory to acknowledge MetaCentrum when using it) in publications to MetaCentrum, and lowered by intensive usage of the service (the usage is calculated from past month)
- After submission of the task, check in the queue in which state it is sometimes it can't start because of impossible combination of requested resources or so
- User can check load of machines
- For more options read

https://docs.metacentrum.cz/computing/resources/resources/

- Request special CPU (AMD, graphical, ...), e.g. CPU with AVX2
 - -1 select=cpu_flag=avx2
- SSD local storage (e.g. -1 scratch_ssd=1gb)
- Request particular location, ...
- https://metavo.metacentrum.cz/pbsmon2/qsub_pbspro helps with preparation of qsub command

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Common problems with launching the tasks

- Script fails because of wrong PATH or missing file ensure all needed files are transferred and applications receive correct paths
 - Rather do not use absolute paths (starting with /) only relative
- Not all required applications are correctly loaded
 - Check documentation and load all needed applications
 - Names of binaries are sometimes little bit different contain names of versions, etc.
- Estimation of time needed to run the task
 - No really good solution...
 - Make some trials and try to estimate...
 - There are very different CPUs available (with different speeds) it is possible to require particular CPU type (but it reduces number of available nodes...)
- Problems with CPU and memory
 - Hard to estimate...
 - Some applications allow setting number of CPU threads check documentation
 - If using Java application, it often helps to request one more CPU thread for Java itself
 - Limiting memory is problematic, e.g. Java allows java -Xmx8g jar ..., some applications also check documentation

Information	Usa	age	Tasks		Graphical con	nection	More :	services	

Get to task's working directory

- Go to https://metavo.metacentrum.cz/pbsmon2/person and click to list of your tasks and click to selected task
- Search for information **exec_host** (address of node doing the task) and **SCRATCHDIR** (temporal directory for all data and results)
- Sometimes one needs to monitor task progress or influence it
- It is not possible to directly modify running task, but at least check (and possibly modify) input data and see outputs

From any MetaCentrum frontend login to respective node running the task
2 ssh exec_host # No need to specify user name; e.g. mandos9

- ³ # Go to SCRATCH directory
- d Cd SCRATCHDIR # e.g. /scratch/USER/job_12345678.meta-pbs.metacentrum.cz/
- ⁵ # There are working data of currently running task...
- 6 # Check whatever you need... Press Ctrl+D to logout

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Running R tasks on MetaCentrum

- There are only some R packages, to get more create own package library and use it in scripts (see e.g. .libPaths() within R)
- Be careful about paths!
- In the metacentrum.sh script load R, e.g.
 module add r/4.1.3-gcc-10.2.1-6xt26dl and start there R script as

usually R CMD BATCH script.r

- 1 Login to selected front node via SSH and load R module
- 2 Create somewhere new directory for R packages mkdir rpkgs (or use default \sim /R/)
- Start R R and install all R packages needed for the task install them into the rpkgs directory install.packages(pkgs=..., lib="rpkgs")
- In the R script *.r load the packages from the rpkgs directory

library(package=..., lib.loc="/storage/.../rpkgs")

5 Ensure all needed outputs are saved from the R script

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Interactive tasks

- # Secure we can log off in the meantime
- 2 screen # Or tmux
- 3 # Again launch qsub according to actual needs
- 4 # Note "-I" for interactive session and missing script name
- 5 qsub -I -l walltime=1:0:0 -l select=1:ncpus=1:mem=1gb:scratch_local=1gb
- 6 # Wait for job to start... User automatically gets to the computing node
- 7 cd \$SCRATCHDIR # Go to \$SCRATCHDIR work there
- 8 # After we get the interactive task, we are on new server
- 9 # Do needed work...
- ¹⁰ # When done, be sure to copy results to the storage
- n hostname # See where we are we can connect to that server directly
- 12 ssh USER@given.server.cz # User name and password are the same
 - # Server address is output from "hostname"
- 14 # When you logout, the task is done (use screen to secure connection)
 - Work as on normal Linux server...
 - With screen we can disconnect as usually and let tasks run in background

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MetaCentrum task

- Upload to any MetaCentrum fronted files metacentrum_oxalis.sh and oxalis_assembly_6235.aln.fasta from scripts_data.
- See metacentrum_oxalis.sh, be sure you know what it is doing, that you understand every command there.
- **③** If needed, edit **metacentrum_oxalis.sh** (e.g. correct paths).
- ④ Submit the task via qsub.
- 6 Monitor the task with qstat.
- 6 Login with SSH to computing node where the task is running, go to \$SCRATCHDIR and see its progress. Look at output of ps ux. What does it say?
- Wait for the task to be done and explore output (e.g. open the treefile in FigTree).
- 8 If you encounter any error, try to find its source and fix it.

Vojtěch Zeisek (

Linux, command line & MetaCentrum

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Graphical interactive task

- See https://docs.metacentrum.cz/software/graphical-access/
- Download and install TightVNC (Windows installer or Java Viewer)

```
screen # Secure we can log off in the meantime
# Again launch qsub according to actual needs
# Note "-I" for interactive session and missing script name
qsub -I -1 walltime=1:0:0 -1 select=1:ncpus=1:mem=1gb:scratch_local=1gb
# Wait for job to start... User automatically gets to the computing node
# After we get the interactive task, we are on new server
module add gui # We need to add GUI module
gui start --ssh # Start GUI (see above link for details)
gui info # Print information about running VNC sessions - use for TightVNC
```

- Work as on normal Linux desktop (ensure to work in **\$SCRATCHDIR**)...
- It provides limited amount of resources, not suitable for big tasks

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Running VNC



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OnDemand

Applications in web browser

- It allows to run selected interactive applications in web browser
- See https://docs.metacentrum.cz/ondemand/ and https://ondemand.grid.cesnet.cz/
- Applications start in storage/brno3-cerit/home/\$USER/ ensure to have everything needed there



Linux, command line & MetaCentrum

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Jupyter Notebook

- Web service allowing to record code as well as its output for languages like BASH, R, Python, ...
- Convenient for recording and sharing code, interactive work, ...
- Use Jupyter Hub for MetaCentrum users
 - Data are typically in /storage/brno2/home/USER/
- Available also as part of OnDemand (previous slide), or bit experimental CERIT hub, which allows to select custom storage and also custom docker image (see documentation)

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	Bunning under: Debian GWU/Linux 10 (buster)	
	Natrix products: default BLAS: /wwr/lib/x86_64-linux-gnu/atlan/libblas.so.3.10.3	
	LAPACK: /usr/l1b/x84_64-linux-gru/atlas/liblapack.so.3.10.3	
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	(3) LC_TIME=an_US_UTF=8 LC_COLLATE=an_US_UTF=8	
	 [5] LC_MOMETARYven_US.UTF+8 LC_MESSAGES+en_US.UTF+8 LC_SAME+C 	
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Introduction									
Information	Usa	ige	Tasks	Graphical connection		More services			
MetaCer	atrum	، دامی	d						

- MetaCentrum cloud (česky) allows to run complete Linux distribution (Debian, CentOS, ...), where you can install any software, like on any other computer
- Useful e.g. for various testing or applications with very special requirements
- Go to https://cloud.metacentrum.cz/ and see documentation
- Login to running virtual machine requires SSH keys to be set up, access is normally via SSH
- Users must have knowledge about Linux administration and follow all security best-practices
- Setting up more than one virtual machine requires good knowledge about Linux networking (user has single public IP address)

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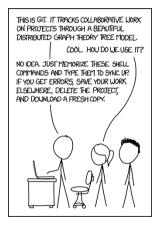
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Introduction						
Git principle		Git basics				

Git

Git Git principle Git basics





https://xkcd.com/1597/

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Git principle		Git basics				

Git and version control I

- Git is version controlling (česky) system (nowadays the most common) it traces changes among all versions absolutely crucial for any software development
- Older (nowadays not so common) version controlling systems is Subversion (SVN); there are many more (Bazaar, Mercurial, ...)
- Probably the best textbook for Git is Chacon's Pro Git
 - Dostupná i česky (včetně prvního vydání)
- Changes and their history is stored in repository (local or network, shared or private) it is possible to view any historical state and differences between any versions
- It is possible to trace who and when did what
- Branching and merging of branches helps with making of big changes
 - When new branch is created, it contains copy of current state
 - User selects in which branch she/he is working, the branches are diverging, user can commit in every branch independently

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Git principle		Git basics				

Git and version control II

- Commits in various branches can be compared and branches can be merged again
- Key feature of Git branches are useful when user starts to work on any big change in the project (the "main" part is intact while developers can freely work on major change)
- Users work on a project in some directory as usually and from time to time commit local changes to staging (temporal area) and then push them to remote or local repository (directory storing all Git history of particular project, can be anywhere)
- Every commit is checkpoint in the history
 - Can be tagged (named), e.g. particular released version of software, or project stage
 - User can compare any two commits or commit and current state
- Stagging area serves as local "container" of changes to be pushed to central Git repository (or to be modified, discarded)
- Central repository keeps whole history of the project
 - Every user has full copy of the central Git repository can be large

Introduction						
Git principle		Git basics				

GitHub and others

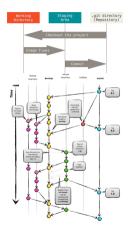
- GitHub is currently probably the most popular platform to host development of open-source projects, see documentation
- Probably second most common on-line service providing Git repository is GitLab
 - User can create an account on GitLab (as on GitHub), or download and install GitLab system on own server (like we did, česky)
- SourceForge used to be more popular in the past, still harbors plenty of interesting projects
- Others are e.g. Bitbucket, Codebase, ...
- For on-line services, many tools are available only for paying customers
- All such services provide Git repositories accessible through standard tools (from command line, see further; or from some special application), through web browser
 - Exact usage might differ from standard Git, check respective help pages first
- Git repository can be easily hosted e.g. on any Linux server...

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Git principle		Git basics				

Git principles

- Three main areas
 - Working directory
 - 2 Staging (changes awaiting to be pushed to central repository)
 - 3 Git repository (remote/local)
- Everyone has whole repository and history (it's "distributed") — very robust
- Flexible branches
 - Very convenient
 - Keeping work structured
 - Separation of tasks
 - Keeping more versions of the project
- Homework: play Oh My Git! to learn more and practice



https://git-scm.com/, https://nvie.com/

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Git principle		Git basics				

Working with Git – start and sending changes

Create a new central repository (e.g. on a server) in empty directory ² git init --bare # No need when establishing project e.g. on GitHub ³ # Create a new repository for new project (in empty directory) 4 git init # No need when cloning from existing repository 5 # If you did not start by cloning, add connection to server ⁶ git remote add origin <location> # Do only once on the beginning 7 # <location> can be remote server or local path ⁸ git remote add origin . # For repository within working directory 9 # Or checkout (make a copy) of existing local or remote repository 10 git clone /path/to/local/repository # Locally mounted repository git clone username@host:/path/to/remote/repository # Over SSH ¹² git clone https://github.com/V-Z/course-linux-command-line-bashscripting-metacentrum.git # Clone from web, e.g. GitHub 13 # Add files to trace with Git 15 # Ignored files (or patterns) can be listed in .gitignore file 16 git add <files> # Or "git add *"

17 git status # See changed files, commits in staging, etc.

Introduction						
Git principle		Git basics				

Working with Git – branching and getting changes

- # Commit changes to prepare them to send to repository
- ² git commit -m "Message..."
- 3 # Push changes into the repository (regardless where it is)
- 4 git push origin master # See further for selection of branches
- 5 # Making new branch and switching to it
- 6 git checkout -b NewFeature # Now we are in branch NewFeature
- 7 # Switch back to branch master
- 8 git checkout master # Generally, "git checkout <branch>"
- 9 # Delete the branch (changes there are lost, must be in another branch)
- 10 git branch -d NewFeature # Delete local branch
- n git push origin --delete <branch> # Delete remote branch
- 12 # New branch must be also pushed to the remote server
- 13 git push origin <branch>
- 14 # List branches (current is marked by asterisk on the beginning)
- 15 git branch
- ¹⁶ # Download news from central server (work of colleagues, etc.)
- 17 git fetch # Downloaded to staging, not applied yet to local files

Introduction						
Git principle		Git basics				

Working with Git – tags, logs and more

- # Update local repository to the newest version from central repository
- ² git pull # Fetch and merge remote changes (before commit)
- $_3$ # Merge another branch into the current one
- 4 git merge <branch>
- 5 # In case of conflict, git shows editor and user must fix it manually
- 6 git add <file with conflict> # Needed to re-add conflicting file
- 7 # To see changes before merging
- 8 git diff <source_branch> <target_branch>
- 9 # Tagging e.g. milestones, released versions of software, etc.
- ¹⁰ git tag <name> <commit id> # <name> can be custom, <commit id> from log:
- " git log # Newest is on top, see also "git log --help"
- 12 git log --graph --oneline --decorate --all # Full long log
- ¹³ # Discard local changes for particular file
- 14 git restore <file>
- 15 # Discard all local changes
- ¹⁶ git fetch origin # Overwrite local changes
- 17 git reset --hard origin/master # If local repository is broken...

Git principle		Git basics				

Working with Git – summary, settings and more

- Basically repeat in git add, commit and push to get your work to the repository, and fetch and pull to download news from central repository
- **diff** to see local changes, **status** to see state
- log and branch show history and branches
- branch, checkout and merge for branching code and merging changes back to master (main) branch

1	git diff # See changes in particular text files
2	gitk # Graphical interface
3	git config color.ui true # Set output to be colored
4	git config format.pretty oneline # Nicer log output
5	<pre>~/.git # Contains user's settings, .git in every repository contains</pre>
6	<pre># data and settings for particular repository</pre>
7	<pre># Default behavior of Git can be heavily altered</pre>

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Git principle		Git basics				
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Git tasks

- git clone https://students:glpat-ms4sHCxhfJBBxUiiu388@git.sorbus.ibot.cas .cz/restio/dadaism.git # It is one long line (no space after .cas)
 - ① Clone the repository using access token (see above) and go to the dadaism directory.
 - 2 Communicate with others to avoid conflicting edits.
 - 3 Add some text files, edit existing text files. Do not add images or another non-text files, do not add large files.
 - **4** Push your changes back to the repository.
 - 5 Fetch changes done by others.
 - 6 See history of changes, who did what, etc.
 - Use at least git commands clone, diff, status, add, commit, push, fetch, pull, log and gitk.
 - 8 You can try to play with branches branch, checkout, merge.

System services					

Administration

AdministrationSystem services



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Managing system services

- Different among distributions several main methods
- In Linux, most common is SystemD, less common older init scripts and RC scripts
- macOS and various BSD and other systems have different methods
- Used to manage system services like networking, cron, web server, database, ...
- Read documentation of your distribution first!
- Most of actions require root authentication
- For SystemD there are also graphical managers (YaST, Systemd-kcm for KDE, GTK Systemd Manager, web-based Cockpit, ...)
- # SystemD huge amount of possibilities
- 2 systemctl enable/disable/status/start/stop servicename # TAB helps
- # RC scripts
- 4 rcservicename status/start/stop # TAB helps to select service
- 5 # Init scripts
- 6 /etc/init.d/servicename status/start/stop # TAB helps to select service

System services					

SystemD usage (few examples)

- # List installed services and their status
- 2 systemctl list-units --type service
- 3 # Enable/disable/see status/start/stop/restart/... service
- 4 systemctl enable/disable/status/start/stop/restart servicename # TAB...
- 5 # Show overridden config files after upgrade
- 6 systemd-delta
- 7 # Analyze boot time (how long does each service take to start)
- 8 systemd-analyze blame # Text output
- 9 systemd-analyze plot > filename.svg # Same in graphics
- 10 # Log for particular service
- n journalctl -u servicename
- 12 # Last logged messages (press Ctrl+C to exit)
- 13 journalctl -f
- 14 # Log records since last boot
- 15 journalctl -b
- 16 # Time and date information and management
- 17 timedatectl

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Resources		The	very end			

The End

The EndResourcesThe very end

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Resources to learn to work in the terminal I

- openSUSE (general handbook) https://doc.opensuse.org/documentation/leap/startup/html/ book-startup/part-bash.html
- Ubuntu (general handbook) https://help.ubuntu.com/community/UsingTheTerminal
- BASH full reference manual https://www.gnu.org/software/bash/manual/(advanced)
- Debian (general handbook) https: //www.debian.org/doc/manuals/debian-reference/ch01.en.html
- Guide to Unix https://en.wikibooks.org/wiki/Guide_to_Unix
- BASH for beginners https://tldp.org/LDP/Bash-Beginners-Guide/ html/Bash-Beginners-Guide.html (the site has plenty of good resources)

Introduction Linux UN*X Command line Text Scripting Software MetaCentrum Git Administration The End Resources The very end

Resources to learn to work in the terminal II

- Grymoire for UNIX wizards https://www.grymoire.com/Unix/
- Linux tutorial https://ryanstutorials.net/linuxtutorial/
- Getting Started with BASH https://www.hypexr.org/bash_tutorial.php
- Bash Guide https://mywiki.wooledge.org/BashGuide
- TutorialKart https://www.tutorialkart.com/bash-shell-scripting
- Česky
 - Učebnice Linuxu https://www.abclinuxu.cz/ucebnice
 - Příkazová řádka Ubuntu https://wiki.ubuntu.cz/syst%C3%A9m/p%C5%99% C3%ADkazov%C3%A1_%C5%99%C3%A1dka/termin%C3%A11
 - Příkazová řádka Fedory https: //wiki.mojefedora.cz/doku.php?id=navody:prirucka:prompt
 - Johančiny Pohádky z příkazové řádky https://eldar.cz/kangaroo/ binarni-sxizofrenie/johanka-pohadky-z-prikazove-radky.html

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Resources		The	very end			

How to ask for help I

- Never ever ask simple silly lazy questions you can quickly find in manual or web
- People on mailing lists and forums respond voluntarily in their spare free time do not waste it be polite, brief and informative
- Imagine you should answer which information do you need?
- Be as specific and exact as possible
 - Write exactly what you did ("It doesn't work!" is useless...)
 - Copy/paste your commands and their output, especially error messages they are keys to solve the problem
 - Try to search web for the error messages (or their parts)
 - Try to provide minimal working example add at least part of your data (if applicable) so that the problem is reproducible
 - Specify name and version of distribution and of the problematic software

• OSS is free as freedom of speech – not as free beer!

• As soon as you don't pay for support, you can't blame anyone for lack of responses

Resources		The	very end			

How to ask for help II

- Most of software we use to process our data is provided under "best effort", without warranty...
- Plenty of scientific software is not written by professional programmers, authors often do not foresee everything what could happen and they could have troubles when fixing reported issues...
- There are plenty of reasons some software doesn't work usage/data author didn't expect, unsupported version of operating system, author's mistake, user's mistake, unexpected interaction with another software, ...
- Authors wish their software to be useful constructive feedback, reporting bugs and wishes is welcomed, but it must be provided in the way useful for the developer
- Try to find the best place to ask your question specific forum for particular distribution or software use to be the best option
- Learning command line is like learning foreign language it takes time...
- Reading documentation is not wasting of time!

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Resources		The	very end			

ChatGPT and others

- Usage of generative AI, large language models (LLM) like ChatGPT can help a lot
- Very good to improve code and fixing non-working code
- Can well explain existing code good starting point
- Good for adaptation of existing code for user's needs
- Limited usage to generate new code can misunderstand request, code can be technically correct, but not well working, can be incomplete or limited in corner-cases
- Without at least basic understanding of subject it is hard to realize if ChatGPT solution is correct user should be at least basically able to work without AI, otherwise there is high risk of failures
- One should never rely on tool with unclear functionality and problematic usage of of users' data and copyrighted content

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Resources		The	very end			

Main general fora I

Question must have certain form!

Before asking, ensure your question is in answerable form (previous slides).

- Sloppily asked question can't be answered at all...
- Check documentation, manuals and search the Internet before asking
- Probably the best are fora from StackExchange https://stackexchange.com/sites
- General forum for programmers https://stackoverflow.com/
- UNIX forum https://unix.stackexchange.com/
- Forum for administrators https://superuser.com/
- Questions mainly (not only) related to servers https://serverfault.com/
- Uncle Google is your friend here ("how to XXX in BASH/Linux") ...

Resources		The	very end			

Main general fora II

- Bioinformatics and related topics is discussed on Biostars and StackExchange
- Do not hesitate to ask on the forum or contact developers, preferably through some public forum or mailing list, they usually respond quickly and helpfully... they wish their software to be working and useful
- Plenty of bigger projects have their own web fora or e-mail conferences search for it to ask on right place
- In Linux/OSS world, e-mail conferences are sometimes more popular, than web forums or various social networks try them
- If you find a bug, report it according to instructions given by the project
- Plenty of software packages have bug (issue) trackers (e.g. on GitHub) to report any problem with the software and discuss search them on software homepage
- Programming languages like R or Python have their own discussion fora, commonly specific for particular field

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openSUS	E					

- Homepage https://www.opensuse.org/
- Wiki (knowledge base) https://en.opensuse.org/Main_Page
- Documentation https://doc.opensuse.org/
- News https://news.opensuse.org/, blogs https://planet.opensuse.org/
- Forums https://forums.opensuse.org/
- Mailing lists https://lists.opensuse.org/
- Community https://opensuse-community.org/, short community guide https://opensuse-guide.org/

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Debian, Ubuntu, Linux Mint and derivatives

- Debian https://www.debian.org/
 - Documentation, wiki https://wiki.debian.org/
 - Support https://www.debian.org/support
- Ubuntu https://ubuntu.com/
 - Support https://ubuntu.com/support
 - Ask Ubuntu (probably the best forum) https://askubuntu.com/
 - Forum https://ubuntuforums.org/
 - Documentation https://help.ubuntu.com/
 - Kubuntu https://kubuntu.org/
 - Kubuntu forum https://www.kubuntuforums.net/
 - Xubuntu https://xubuntu.org/
 - Lubuntu https://lubuntu.me/
- Linux Mint https://www.linuxmint.com/
 - Documentation https://www.linuxmint.com/documentation.php
 - Forums https://forums.linuxmint.com/

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Fedora						

- Homepage https://fedoraproject.org/
- Communication and help overview https: //fedoraproject.org/wiki/Communicating_and_getting_help
- Wikihttps://fedoraproject.org/wiki/Fedora_Project_Wiki
- Official forum https://discussion.fedoraproject.org/
- Documentation https://docs.fedoraproject.org/
- Community forum https://fedoraforum.org/

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GNOME, KDE and XFCE

- GNOME https://www.gnome.org/
 - Help for users https://help.gnome.org/users/
 - Wikihttps://wiki.gnome.org/
- KDE https://kde.org/
 - Forum https://discuss.kde.org/
 - UserBase wiki https://userbase.kde.org/
 - Application store https://store.kde.org/
 - KDE for education https://apps.kde.org/categories/education/
 - Blogs https://planet.kde.org/
- XFCE https://xfce.org/
 - Documentation https://docs.xfce.org/
 - Wiki https://wiki.xfce.org/
 - Forum https://forum.xfce.org/
 - Blogs https://blog.xfce.org/

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LibreOff	ice					

- LibreOffice https://www.libreoffice.org/
 - Document Foundation https://www.documentfoundation.org/
 - Ask LO https://ask.libreoffice.org/
 - Wiki of LO https://help.libreoffice.org/ and DF https://wiki.documentfoundation.org/Main_Page
 - Documentation https://documentation.libreoffice.org/
- Česky
 - Novinky a informace https://www.openoffice.cz/
 - Fórum https://forum.openoffice.cz/
 - Podrobná příručka https:

//www.root.cz/knihy/libreoffice-writer-prakticky-pruvodce/
(jedna z vůbec nejlepších dostupných knih)

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České weby – zdroje informací a fóra l

- ABC Linuxu https://www.abclinuxu.cz/
 - Učebnice GNŪ/Linuxu https://www.abclinuxu.cz/ucebnice
- Root https://www.root.cz/
- LinuxExpres https://www.linuxexpres.cz/
 - Správa linuxového serveru https://www.linuxexpres.cz/praxe/sprava-linuxoveho-serveru
- LinuxDays (největší konference) https://www.linuxdays.cz/
- Seminář Install fest https://installfest.cz/
- Konference OpenAlt https://openalt.cz/
- OpenOffice/LibreOffice https://www.openoffice.cz/
 - Podrobná příručka https:

//www.root.cz/knihy/libreoffice-writer-prakticky-pruvodce/

- Fórum https://forum.openoffice.cz/
- Ubuntu https://www.ubuntu.cz/

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Resources		The	very end			

České weby – zdroje informací a fóra II

- Wiki https://wiki.ubuntu.cz/
- Fórum https://forum.ubuntu.cz/
- Fedora https://mojefedora.cz/
 - Wiki https://wiki.mojefedora.cz/doku.php
 - Fórum https://forum.mojefedora.cz/
 - Příručka

https://wiki.mojefedora.cz/doku.php?id=navody:prirucka:obsah

- Linux Mint https://www.linux-mint-czech.cz/
 - Fórum https://forum.linux-mint-czech.cz/
- Johančiny Pohádky z příkazové řádky https://eldar.cz/kangaroo/ binarni-sxizofrenie/johanka-pohadky-z-prikazove-radky.html

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...I hope it was helpful for You...

...any feedback is welcomed...

...happy Linux hacking...

...any final questions?

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Vojtěch Zeisek (https://trapa.cz/)	Linux, command line & MetaCentrum	January 14 to 16, 2025	317 / 317