CENTRO DE ANÁLISIS DE DATOS Y SUPERCÓMPUTO

CADS

INTRODUCCIÓN A AMBIENTES HPC: Linux

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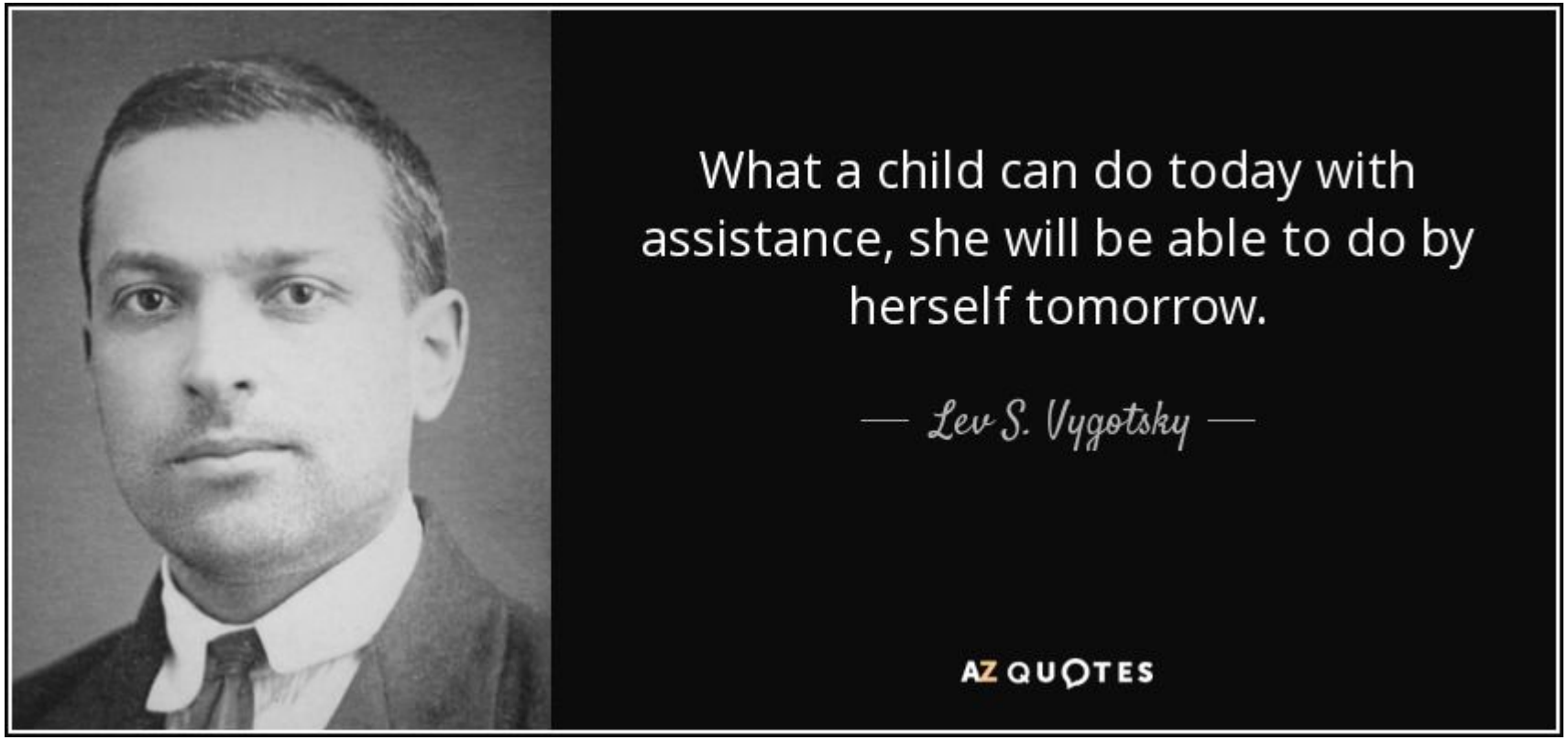
Red Universitaria e Institución Benemérita de Jalisco

CGSTIC

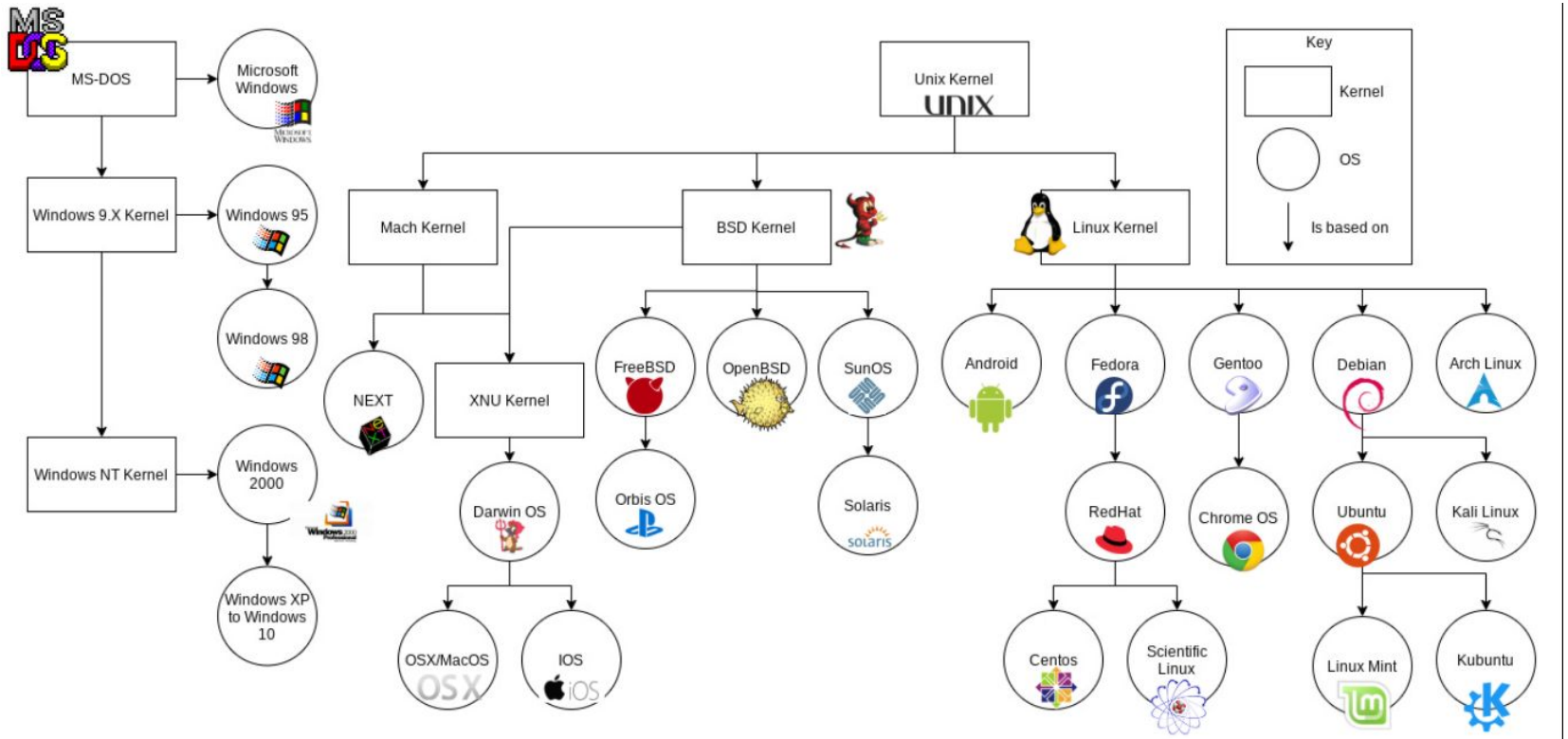
Coordinación General de Servicios Administrativos e Infraestructura Tecnológica


What a child can do today with assistance, she will be able to do by herself tomorrow.
— Lev S. Vygotsky —
AZ QUOTES

Contenido

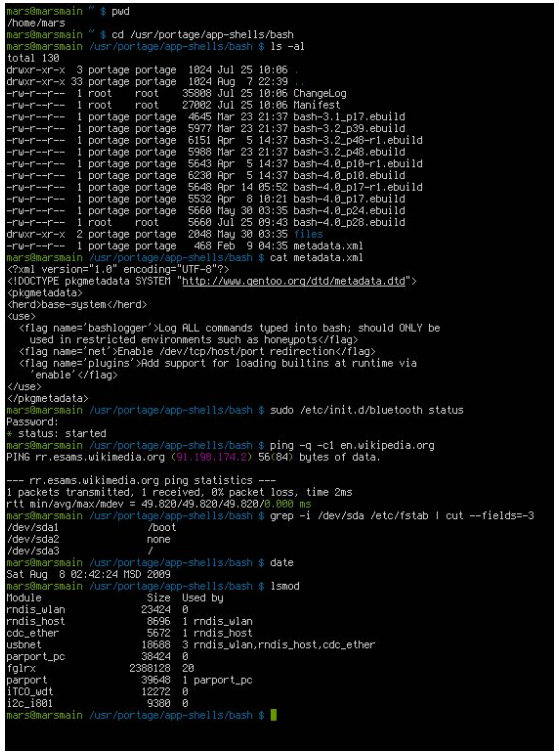
- Introducción qué es HPC
- Sistemas Operativos (CLI/GUI)
- Linux
- Conexión shh e interfaces
- Aplicaciones en Leo Átrox
- Comandos básicos en Linux
- Edición de archivos

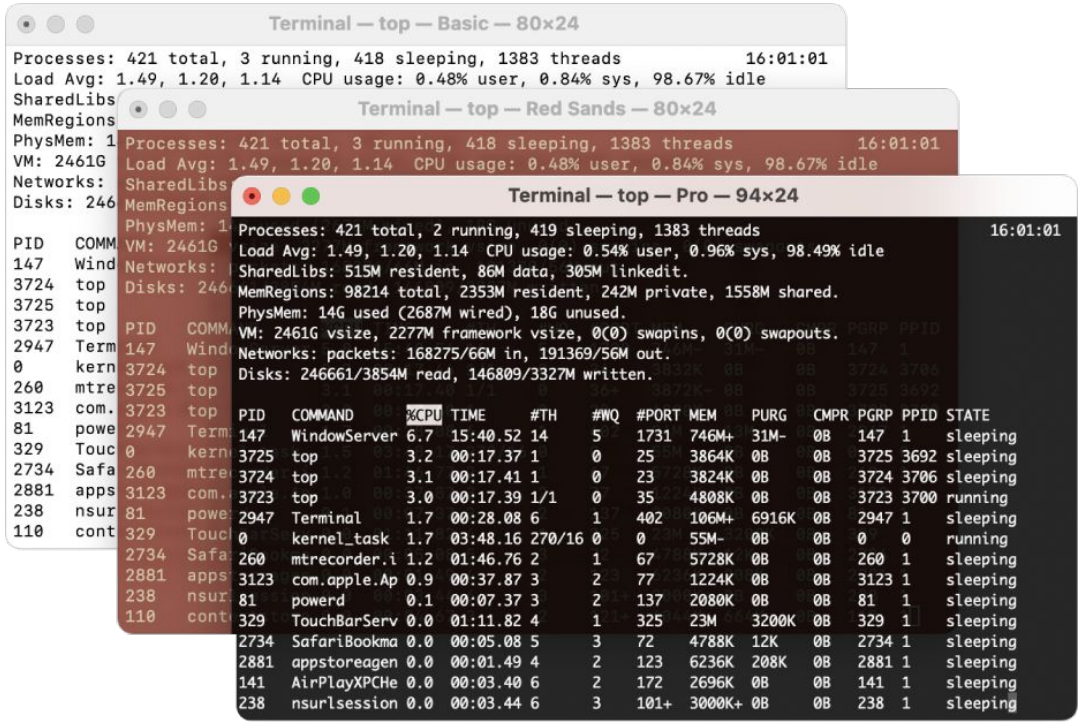
Sistemas operativos

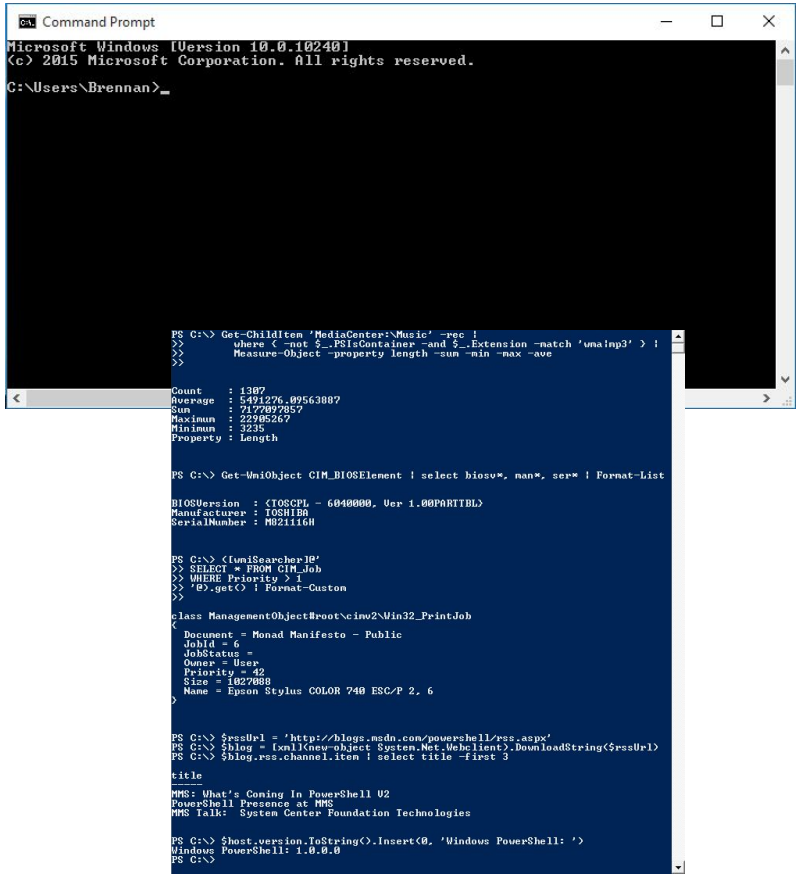


https://i.imgur.com/EpT5Pwf.png

Command line Interface (CLI)







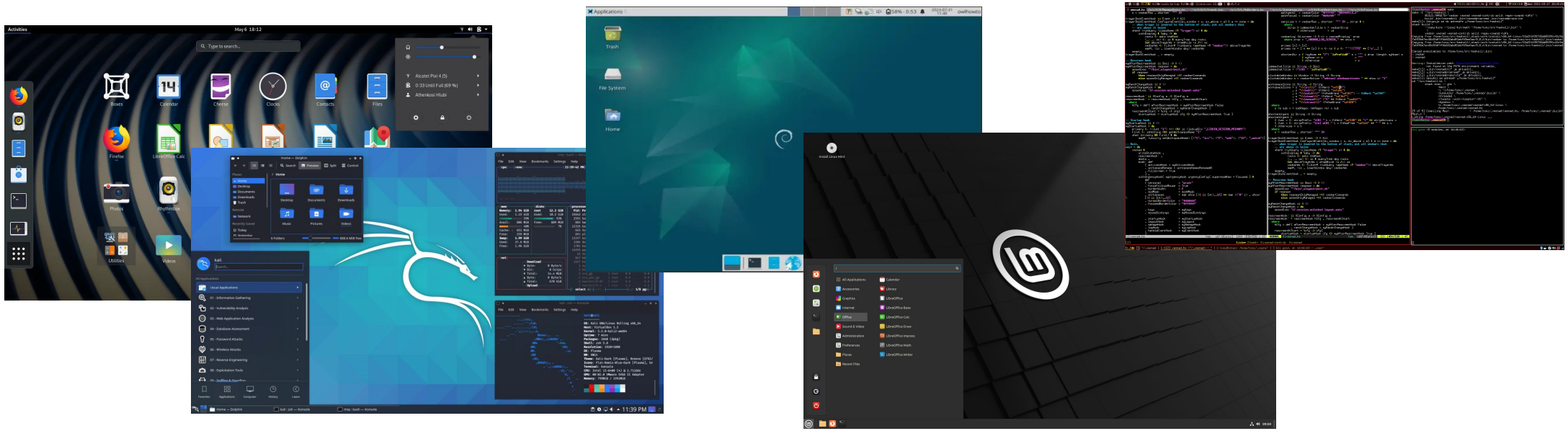
https://es.wikipedia.org/wiki/S%C3%ADmbolo_del_sistema_de_Windows
https://es.wikipedia.org/wiki/Shell_de_Unix
https://support.apple.com/es-es/guide/terminal/trml2df0220c/mac

Shell

- La shell es un intérprete de comandos. Estos traducen el lenguaje escrito para que el sistema operativo lo entienda.
- Se llama shell denota una capa externa de interacción entre el usuario y sistema operativo.

https://rsg-ecuador.github.io/unix.bioinfo.rsgecuador/content/Curso_basico/03_Manejo_terminal/1_def.html

GUI (Graphics User interface)

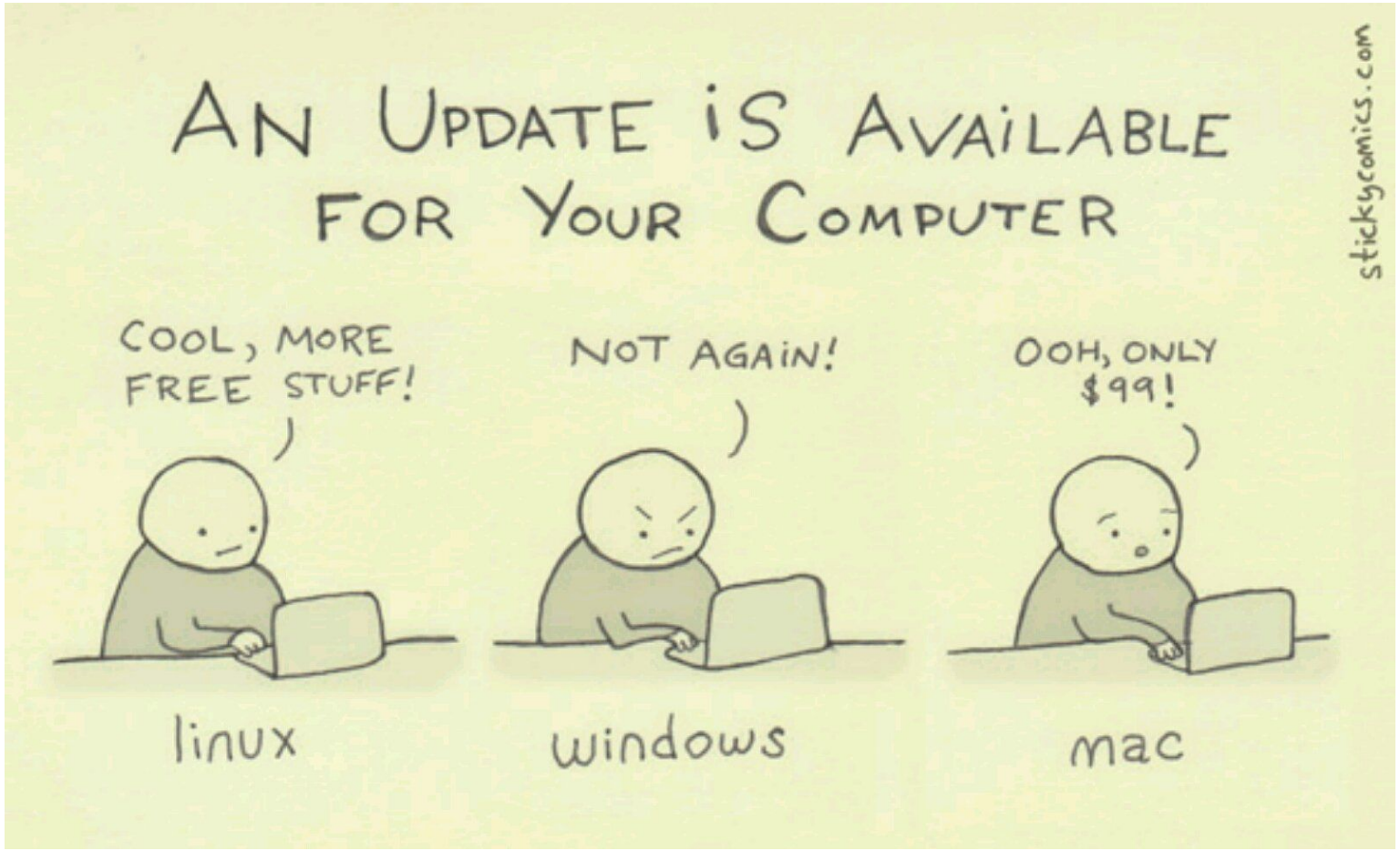


GNOME™

KDE

XFCE

xmonad


AN UPDATE IS AVAILABLE FOR YOUR COMPUTER
stickycomics.com
COOL, MORE FREE STUFF!
NOT AGAIN!
OOH, ONLY $99!
linux
windows
mac

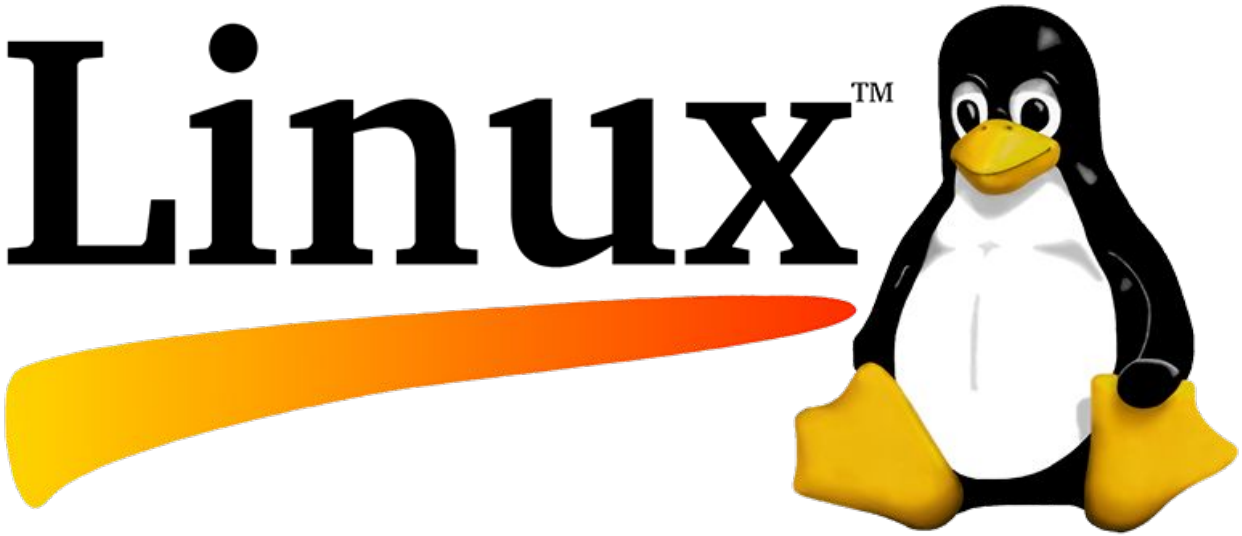
¿Por qué un sistema linux?

Gratuito: no es necesario adquirir una licencia y el código es libre.

Estabilidad: Trabaja muy bien en ambientes de multiusuarios.

Seguridad: Es más seguro que otros sistemas operativos.

HPC: Es el sistema operativo utilizado en las 500 computadoras más potentes del mundo.



Distribuciones famosas para servidor

Red Hat

fedora

AlmaLinux

Rocky Linux™

CentOS

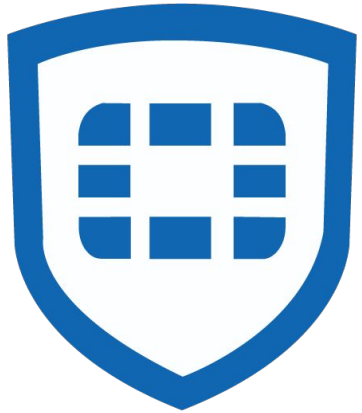
ubuntu

VPN

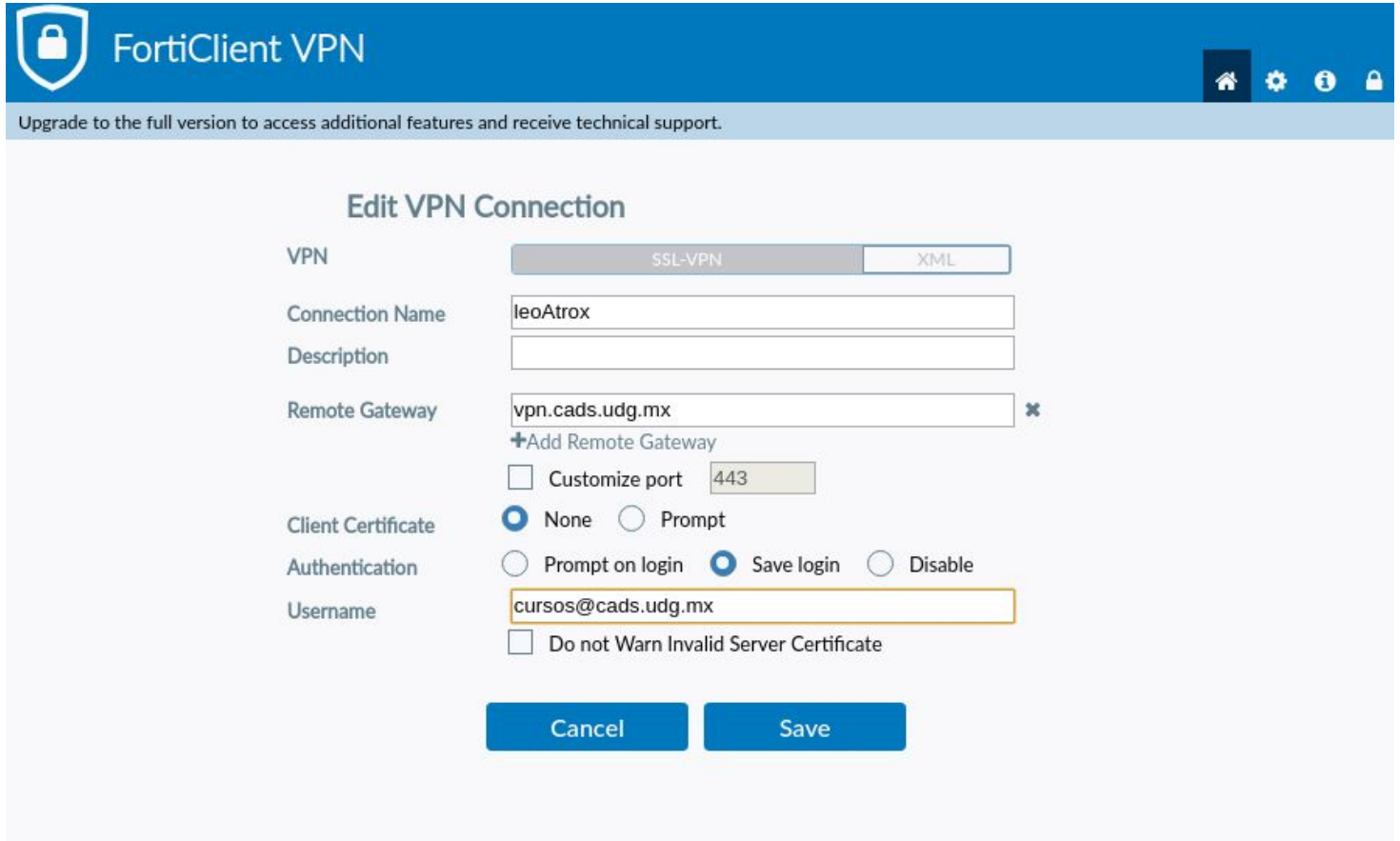
Descargar forticlient:
Linux
https://www.fortinet.com/support/product-downloads
Windows
https://drive.google.com/drive/folders/1IRoUer-d9LUjCmOyXnW8gmezziZ8-wpF?usp=sharing
MAC FortiVPN 6
http://148.202.15.34/files/

Descargar mobaXterm

Windows
https://mobaxterm.mobatek.net/download-home-edition.html



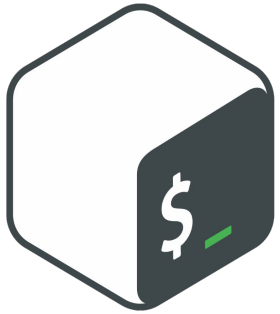
Openfortivpn https://github.com/adrienverge/openfortivpn


FortiClient VPN
Upgrade to the full version to access additional features and receive technical support.
Edit VPN Connection
VPN
SSL-VPN
XML
Connection Name
leoAtrox
Description
Remote Gateway
vpn.cads.udg.mx
+Add Remote Gateway
Customize port
443
Client Certificate
None
Prompt
Authentication
Prompt on login
Save login
Disable
Username
cursos@cads.udg.mx
Do not Warn Invalid Server Certificate
Cancel
Save

Herramientas para conexiones SSH

- PUTTY
- MOBAXTERM
- BITVISE
- TERMINAL

PuTTY



BASH
THE BOURNE-AGAIN SHELL

bitvise

MobaXterm

Transferir archivos vía terminal

```
rsync -vp ~/archivo.txt  [usuario]@login1.cads.udg.mx:/lustre/home/usuario/

rsync -avnr [folder] [usuario]@login1.cads.udg.mx:/lustre/home/usuario
```

bitvise

Filezilla

MobaXterm

Aplicaciones

CODE
Visual Studio Code

jupyter

VSCodium

MATLAB®

EMACS

Conectarse a una sesión remota

Información de la VPN

- **Username:** cursos@cads.udg.mx
- **Contraseña:** 202404.hpc
- **Gateway:** vpn.cads.udg.mx
- **Puerto:** 443

Información de la máquina virtual

- **Dirección IP:** login1.cads.udg.mx
- **Usuario/Hostname:** curso[1-15]
- **Contraseña:** CADS.2023
- **Puerto:** 22

Linux consola

Interfaz: [nombre de usuario][nodo login][directorio home (~)]$

```
[usuario@chn02 ~]$
```

Cómo obtener ayuda:

```
[usuario@chn02 ~]$  man ls
[usuario@chn02 ~]$  help  --ls
```

Interface

pwd : (*power working directory*) ver la el directorio donde estamos trabajando:

```
[usuario@chn02 ~]$  pwd
/lustre/home/usuario
```

$HOME o **~/** :

```
[usuario@chn02 ~]$  $HOME
[usuario@chn02 ~]$  ~/
-bash: /lustre/home/usuario/: Is a director
```

Navegación

Comando	Opciones útiles	Descripción
ls	**ls -l**	Muestra el contenido del directorio como una lista
mkdir		Crea un directorio
cd	**cd ..**	Cambia el directorio de trabajo
rmdir		Borra el directorio vacio
tree		Presenta los directorios en forma de árbol
cp	**-v**	Copia archivos o directorios
mv	**-v**	Mueve archivos o directorios
rm		Borrar archivo o directorio
touch		crear un archivo vacío

Ejercicio

Visualiza el directorio en el que te encuentras actualmente.
Pista. El resultado del comando introducido se ve de la siguiente manera:

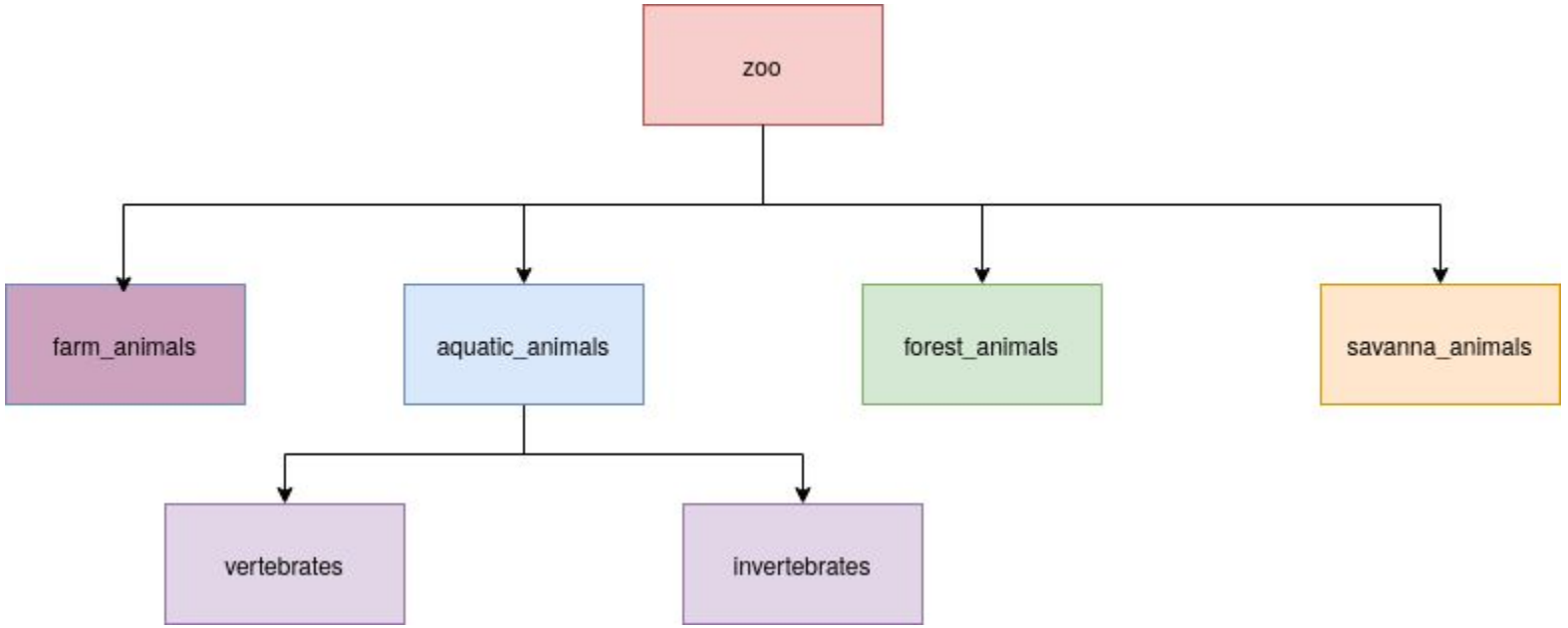
```
/lustre/home/curso1
```

Solución

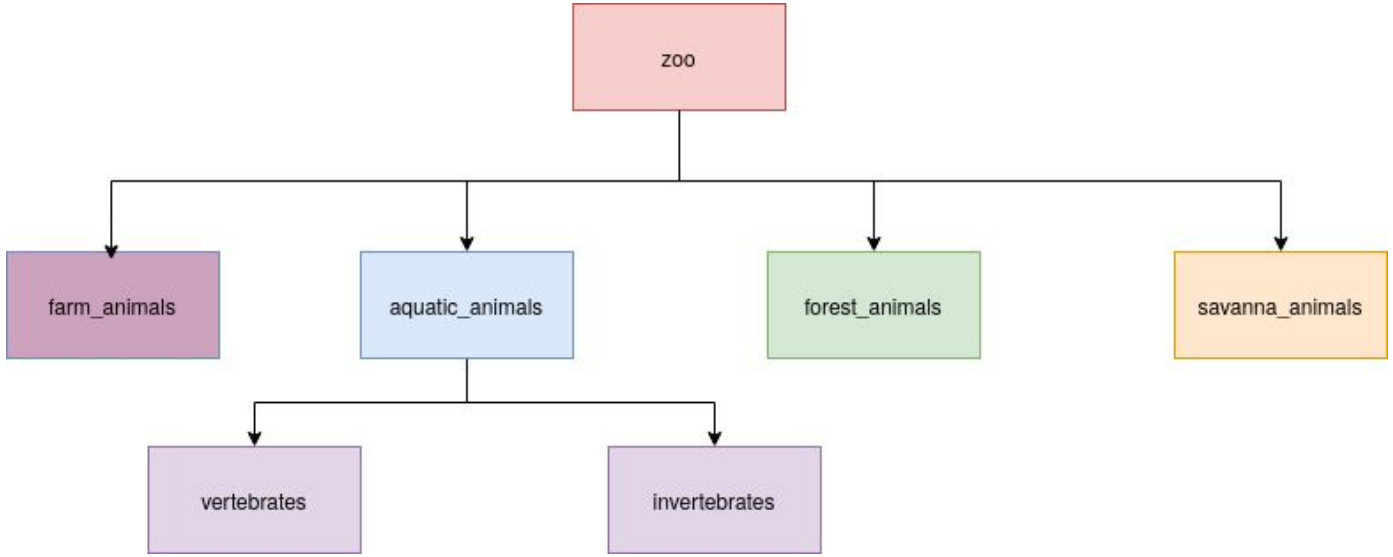
```
[curso1@chn02 ~]$ pwd
/lustre/home/curso1
```

Ejercicio

Usando los comandos anteriores crea la siguiente estructura de directorios:

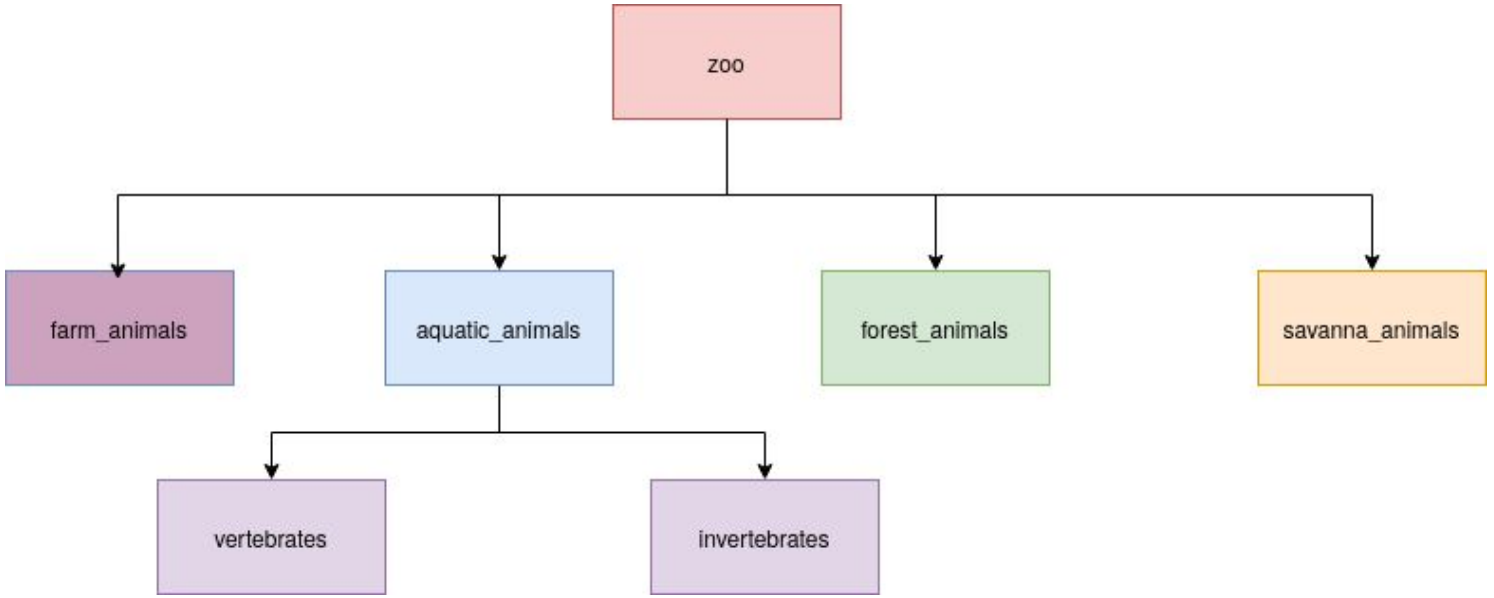


Solución 1




```
omar@ubuntu:~/Documents/presentation$ mkdir zoo
omar@ubuntu:~/Documents/presentation$ mkdir zoo/farm_animals
omar@ubuntu:~/Documents/presentation$ mkdir zoo/aquatic_animals
omar@ubuntu:~/Documents/presentation$ mkdir zoo/aquatic_animals/vertebrates
omar@ubuntu:~/Documents/presentation$ mkdir zoo/aquatic_animals/invertebrates
omar@ubuntu:~/Documents/presentation$ mkdir zoo/forest_animals
omar@ubuntu:~/Documents/presentation$ mkdir zoo/savanna_animals
```

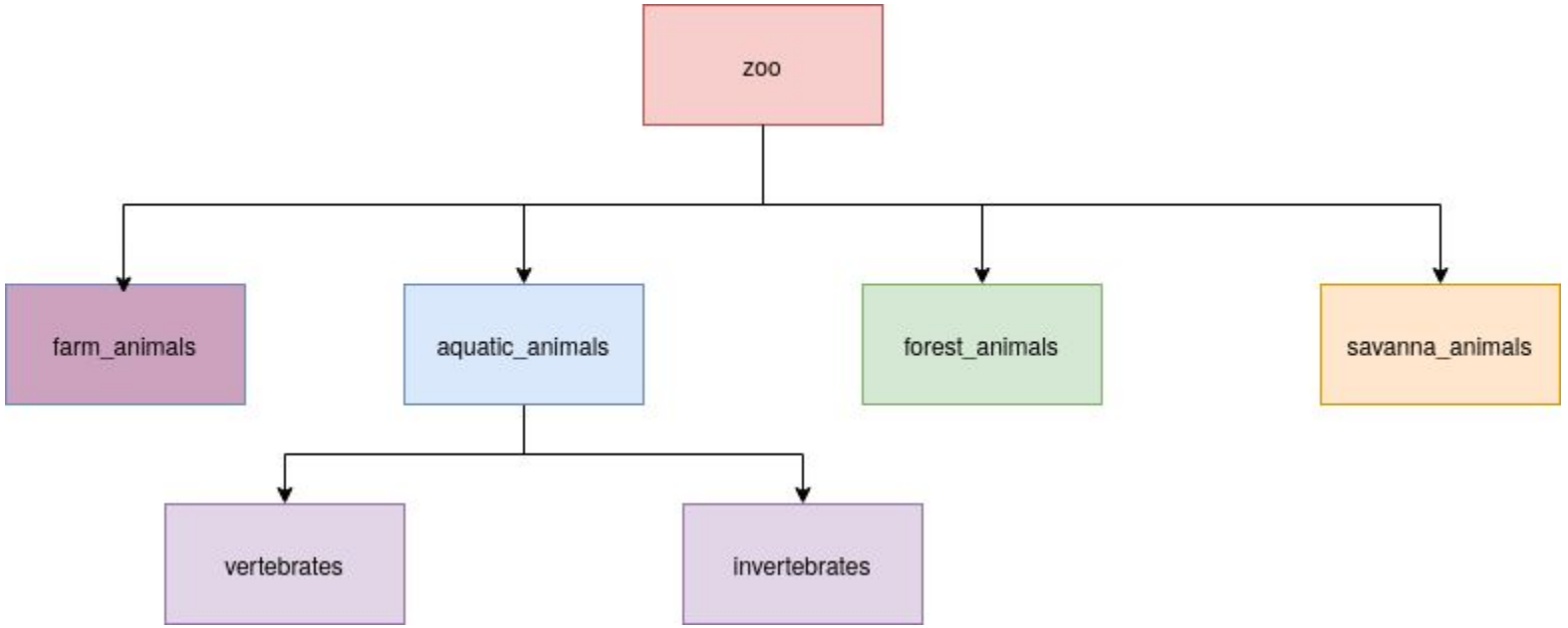
Solución 2



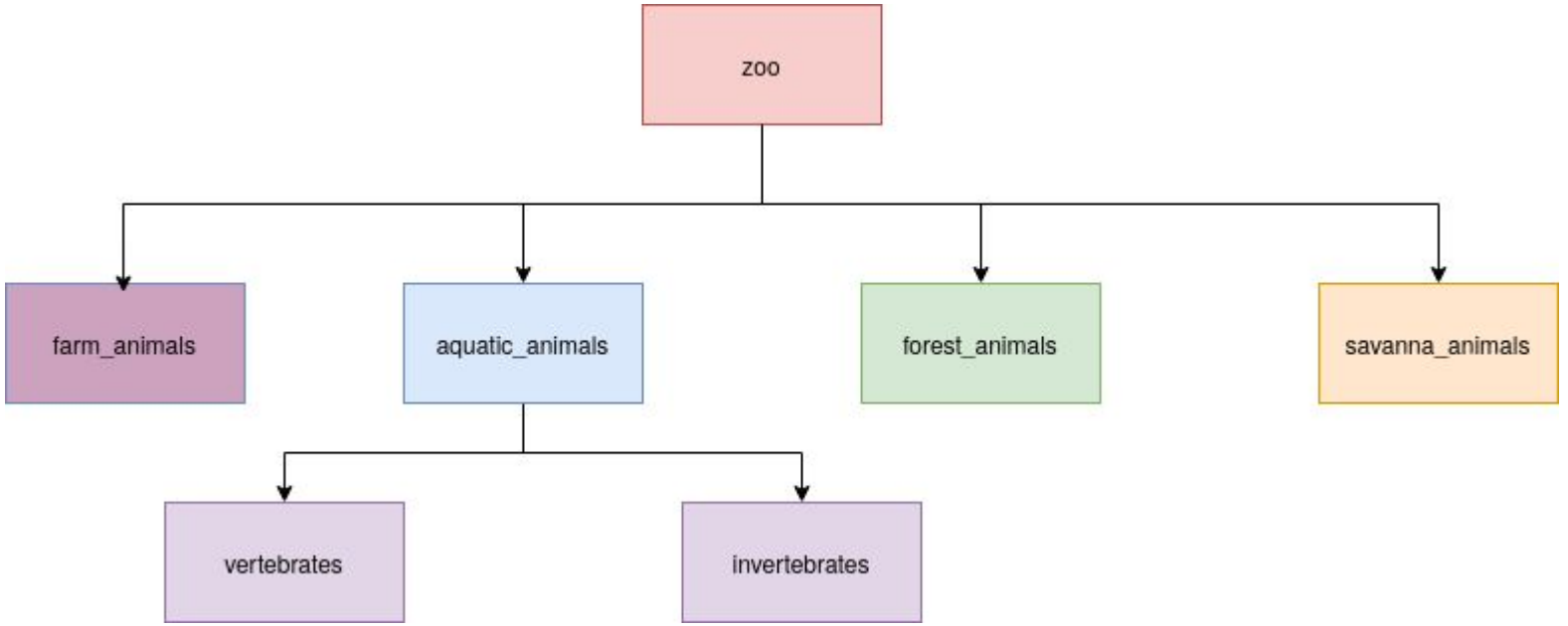

```
(base) omar@ubuntu:~/Documents/presentation$ mkdir zoo zoo/farm_animals zoo/aquatic_animals zoo/aquatic_animals/vertebrates zoo/aquatic_animals/invertebrates zoo/forest_animals zoo/savanna a
nimals
```

Ejercicio

Lista los contenidos de cada directorio.

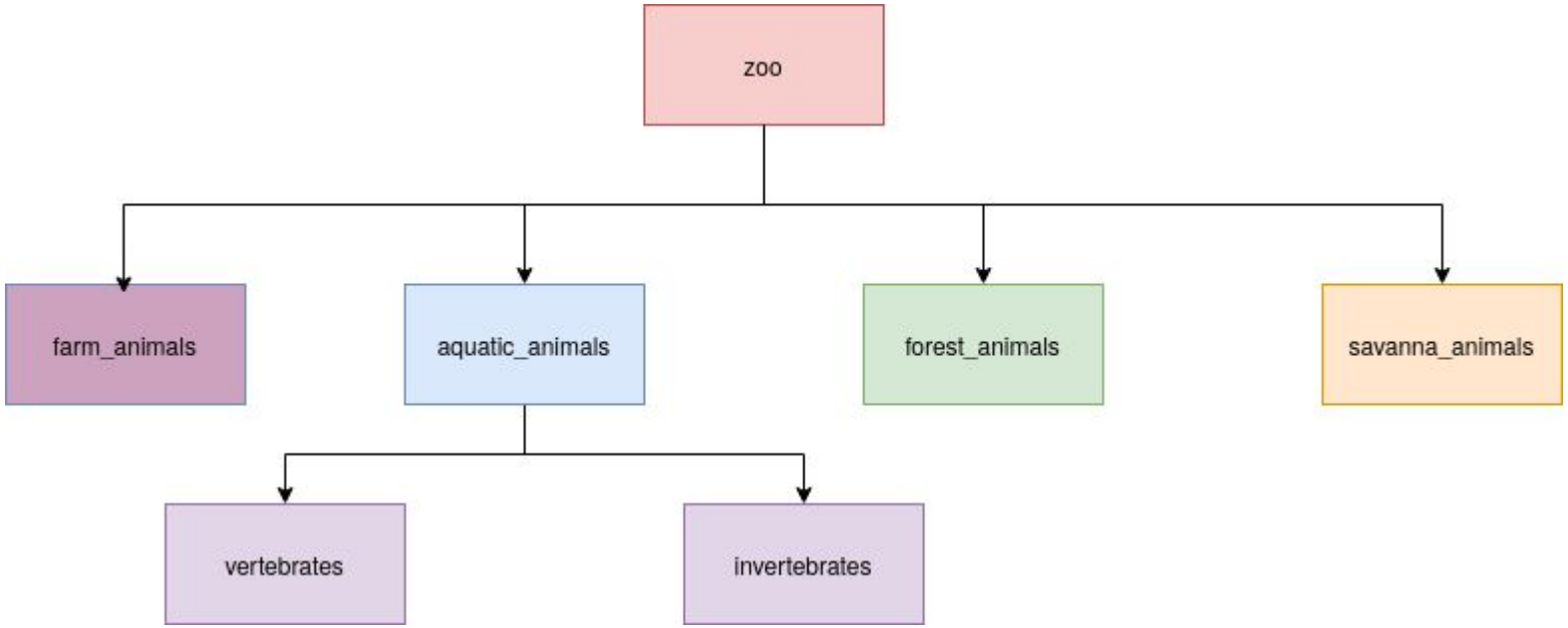


Solución 1




```
(base) omar@ubuntu:~/Documents/presentation$ ls zoo/
aquatic_animals  farm_animals  forest_animals  savanna_animals
(base) omar@ubuntu:~/Documents/presentation$ ls zoo/aquatic_animals/
invertebrates  vertebrates
```

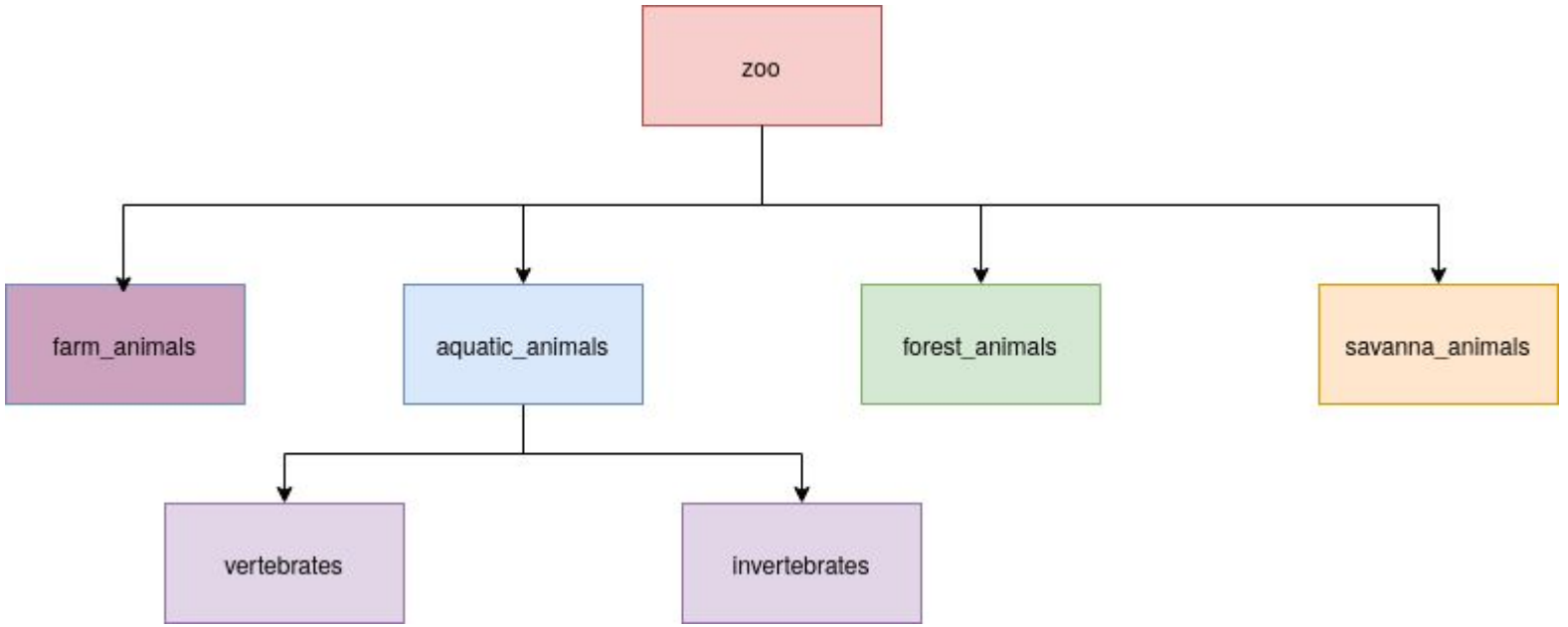
Solución 2



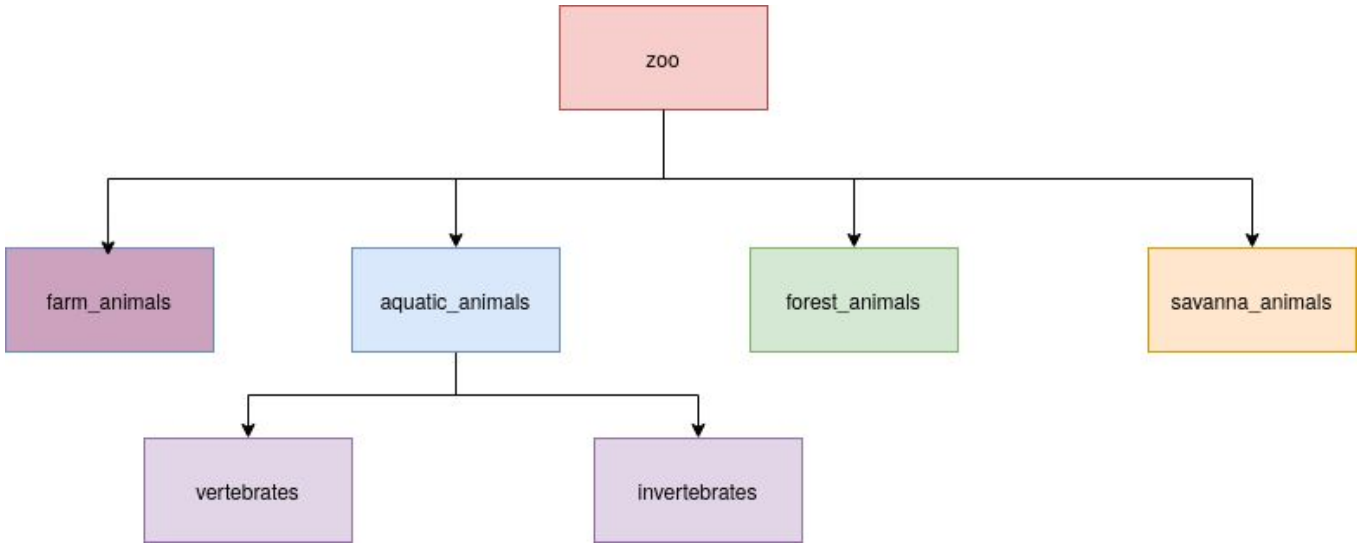

```
(base) omar@ubuntu:~/Documents/presentation$ ls -l zoo/
total 16
drwxrwxr-x 4 omar omar 4096 Oct  4 09:16 aquatic_animals
drwxrwxr-x 2 omar omar 4096 Oct  4 09:16 farm_animals
drwxrwxr-x 2 omar omar 4096 Oct  4 09:16 forest_animals
drwxrwxr-x 2 omar omar 4096 Oct  4 09:16 savanna_animals
(base) omar@ubuntu:~/Documents/presentation$ ls -l zoo/aquatic_animals/
total 8
drwxrwxr-x 2 omar omar 4096 Oct  4 09:16 invertebrates
drwxrwxr-x 2 omar omar 4096 Oct  4 09:16 vertebrates
```

Ejercicio

Navega por la estructura de directorios.



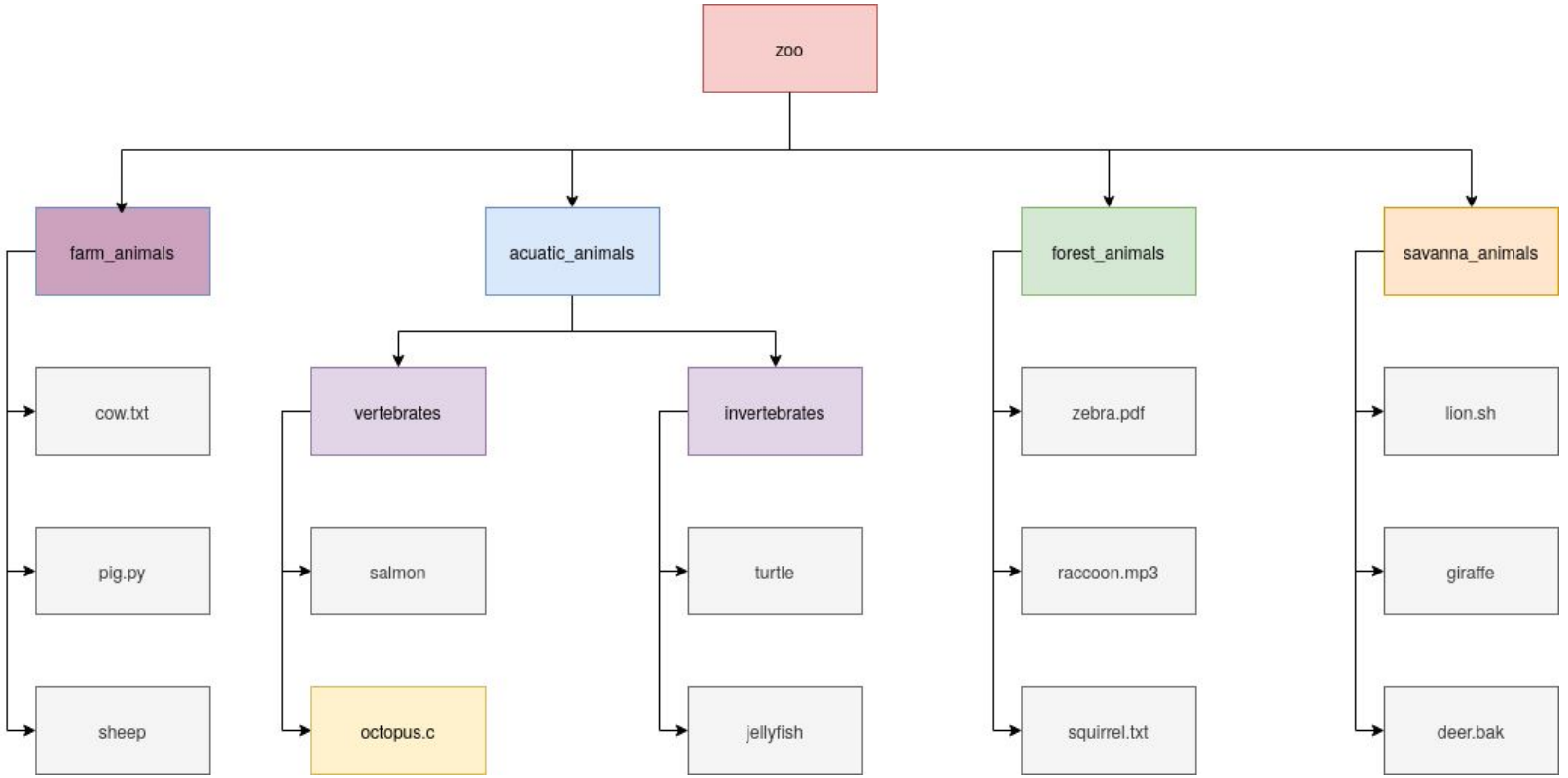
Solución



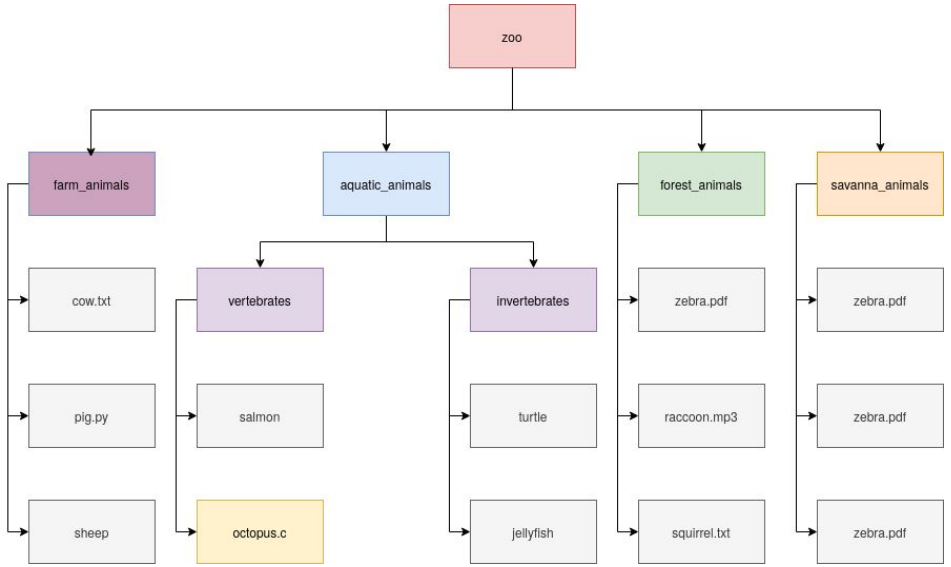

```
(base) omar@ubuntu:~/Documents/presentation$ cd zoo
(base) omar@ubuntu:~/Documents/presentation/zoo$ ll
total 24
drwxrwxr-x 6 omar omar 4096 Oct  4 09:16 ./
drwxrwxr-x 3 omar omar 4096 Oct  4 09:15 ../
drwxrwxr-x 4 omar omar 4096 Oct  4 09:16 aquatic_animals/
drwxrwxr-x 2 omar omar 4096 Oct  4 09:16 farm_animals/
drwxrwxr-x 2 omar omar 4096 Oct  4 09:16 forest_animals/
drwxrwxr-x 2 omar omar 4096 Oct  4 09:16 savanna_animals/
(base) omar@ubuntu:~/Documents/presentation/zoo$ cd aquatic_animals/
(base) omar@ubuntu:~/Documents/presentation/zoo/aquatic_animals$ ll
total 16
drwxrwxr-x 4 omar omar 4096 Oct  4 09:16 ./
drwxrwxr-x 6 omar omar 4096 Oct  4 09:16 ../
drwxrwxr-x 2 omar omar 4096 Oct  4 09:16 invertebrates/
drwxrwxr-x 2 omar omar 4096 Oct  4 09:16 vertebrates/
(base) omar@ubuntu:~/Documents/presentation/zoo/aquatic_animals$ cd ../
(base) omar@ubuntu:~/Documents/presentation/zoo$ cd farm_animals/
(base) omar@ubuntu:~/Documents/presentation/zoo/farm_animals$ cd ..
(base) omar@ubuntu:~/Documents/presentation/zoo$ cd forest_animals/
(base) omar@ubuntu:~/Documents/presentation/zoo/forest_animals$ cd ..
(base) omar@ubuntu:~/Documents/presentation/zoo$ cd savanna_animals/
```

Ejercicio

Crea dentro de la estructura de directorios los siguientes ficheros.



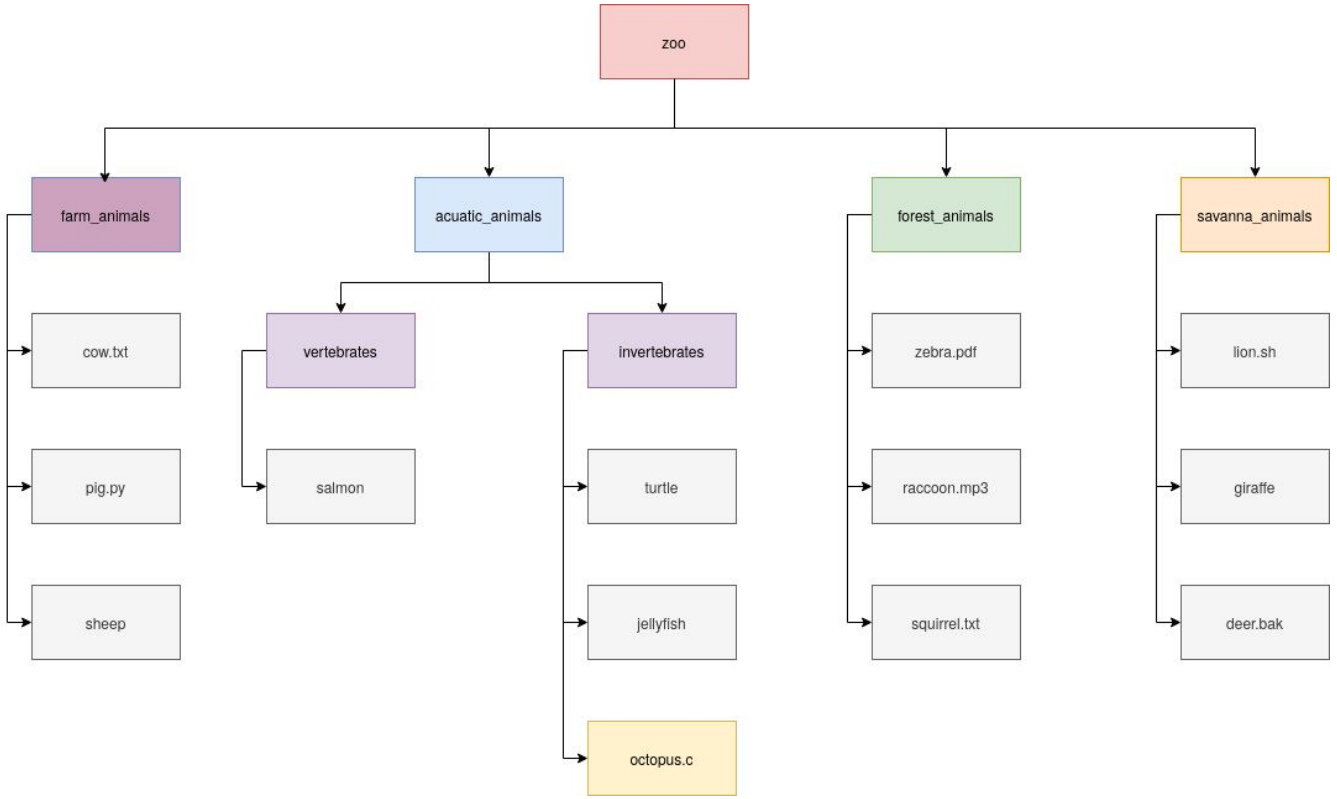
Solución



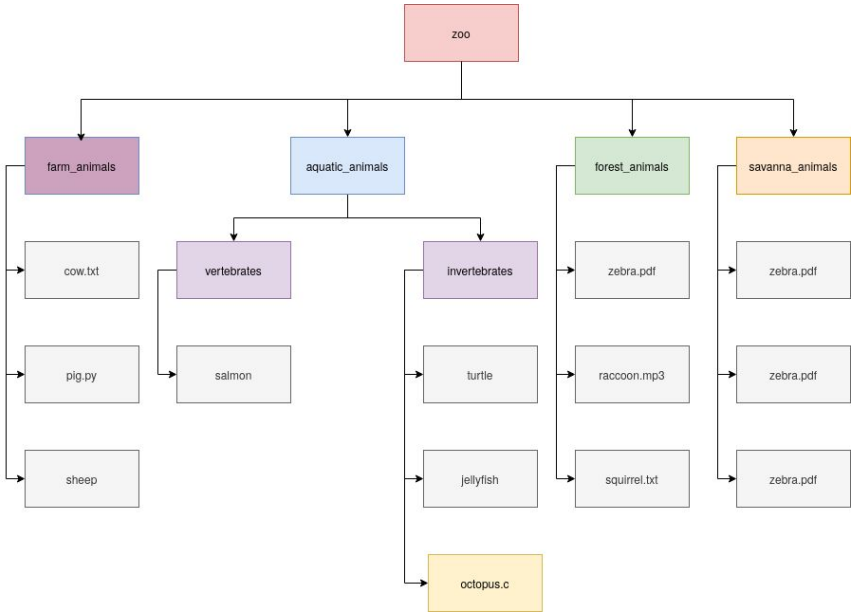

```
(base) omar@ubuntu:~/Documents/presentation/zoo$ cd farm_animals/
(base) omar@ubuntu:~/Documents/presentation/zoo/farm_animals$ touch cow.txt pig.py sheep
(base) omar@ubuntu:~/Documents/presentation/zoo/farm_animals$ cd ..
(base) omar@ubuntu:~/Documents/presentation/zoo$ cd forest_animals/
(base) omar@ubuntu:~/Documents/presentation/zoo/forest_animals$ touch zebra.pdf raccoon.mp3 squirrel.txt
(base) omar@ubuntu:~/Documents/presentation/zoo/forest_animals$ cd ../savanna_animals/
(base) omar@ubuntu:~/Documents/presentation/zoo/savanna_animals$ touch lion.sh giraffe deer.bak
(base) omar@ubuntu:~/Documents/presentation/zoo/savanna_animals$ cd ../aquatic_animals/vertebrates/
(base) omar@ubuntu:~/Documents/presentation/zoo/aquatic_animals/vertebrates$ touch salmon octopus.c
(base) omar@ubuntu:~/Documents/presentation/zoo/aquatic_animals/vertebrates$ cd ../invertebrates/
(base) omar@ubuntu:~/Documents/presentation/zoo/aquatic_animals/invertebrates$ touch turtle jellyfish
```

Ejercicio

Mueve el fichero octopus.c hacia el directorio aquatic_animals/invertebrates.



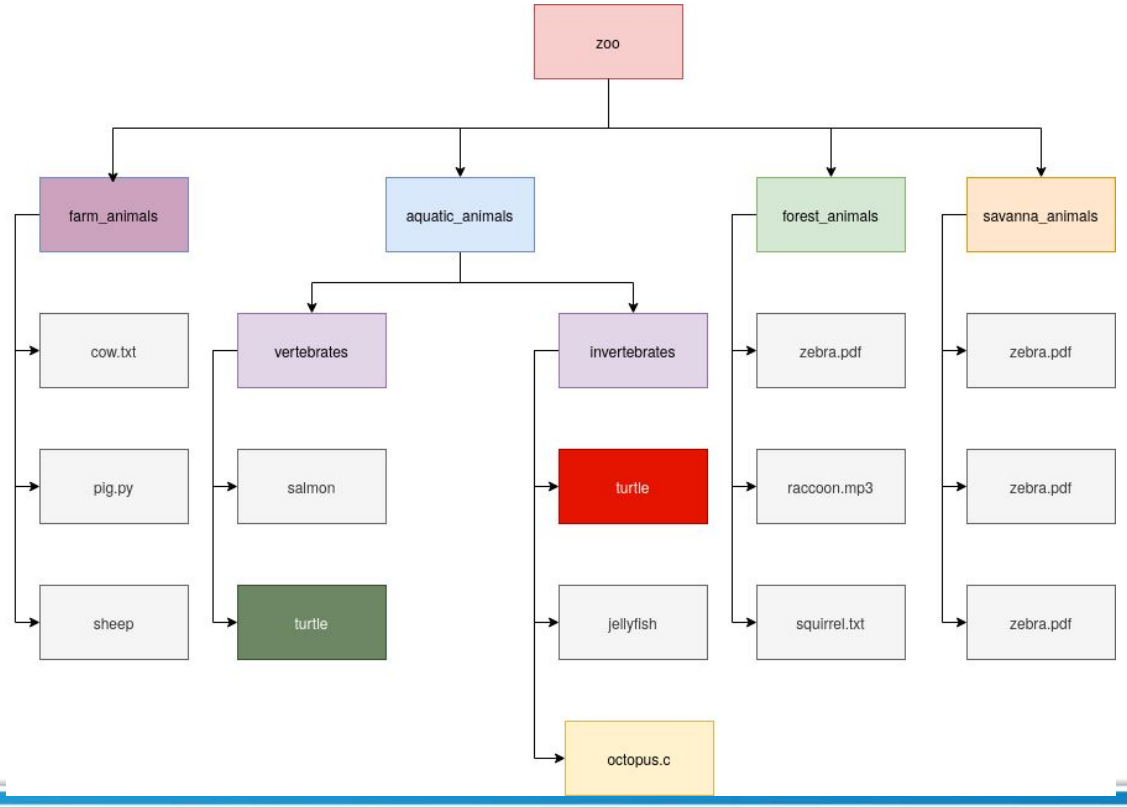
Solución



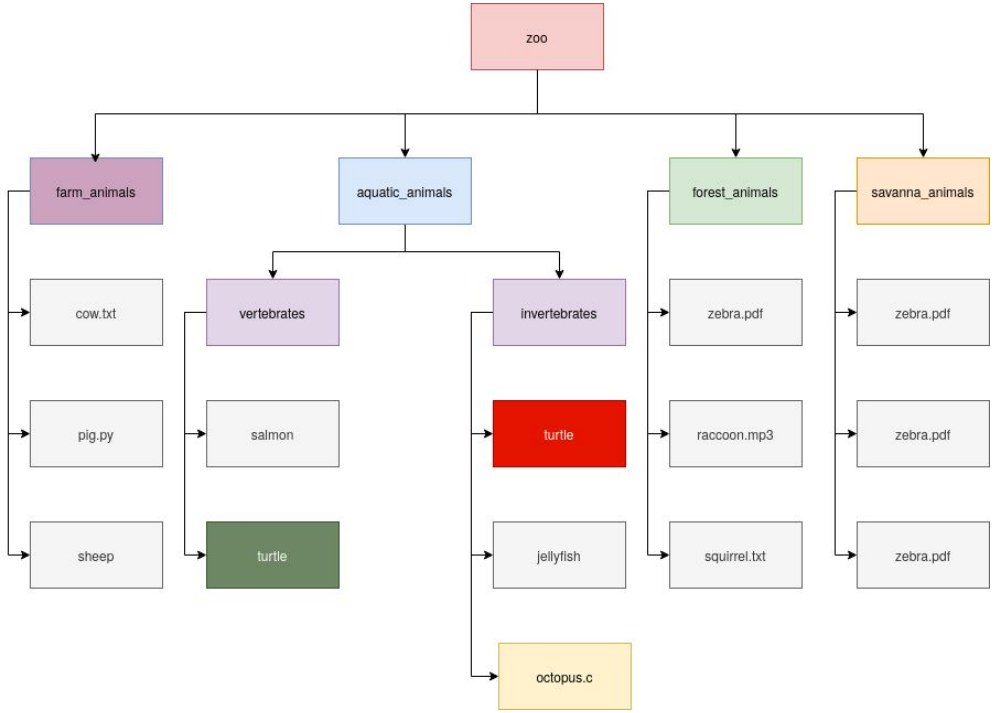

```
(base) omar@ubuntu:~/Documents/presentation/zoo/aquatic_animals/vertebrates$ cd ../..
(base) omar@ubuntu:~/Documents/presentation/zoo$ cd aquatic_animals/vertebrates/
(base) omar@ubuntu:~/Documents/presentation/zoo/aquatic_animals/vertebrates$ mv octopus.c ../invertebrates/
(base) omar@ubuntu:~/Documents/presentation/zoo/aquatic_animals/vertebrates$ ll ../invertebrates/
total 8
drwxrwxr-x 2 omar omar 4096 Oct  4 09:40 ./
drwxrwxr-x 4 omar omar 4096 Oct  4 09:16 ../
-rw-rw-r-- 1 omar omar    0 Oct  4 09:35 jellyfish
-rw-rw-r-- 1 omar omar    0 Oct  4 09:35 octopus.c
-rw-rw-r-- 1 omar omar    0 Oct  4 09:35 turtle
```

Ejercicio

Copia el fichero turtle desde el directorio aquatic_animals/invertebrates hacia aquatic_animals/vertebrates y elimina el fichero original.



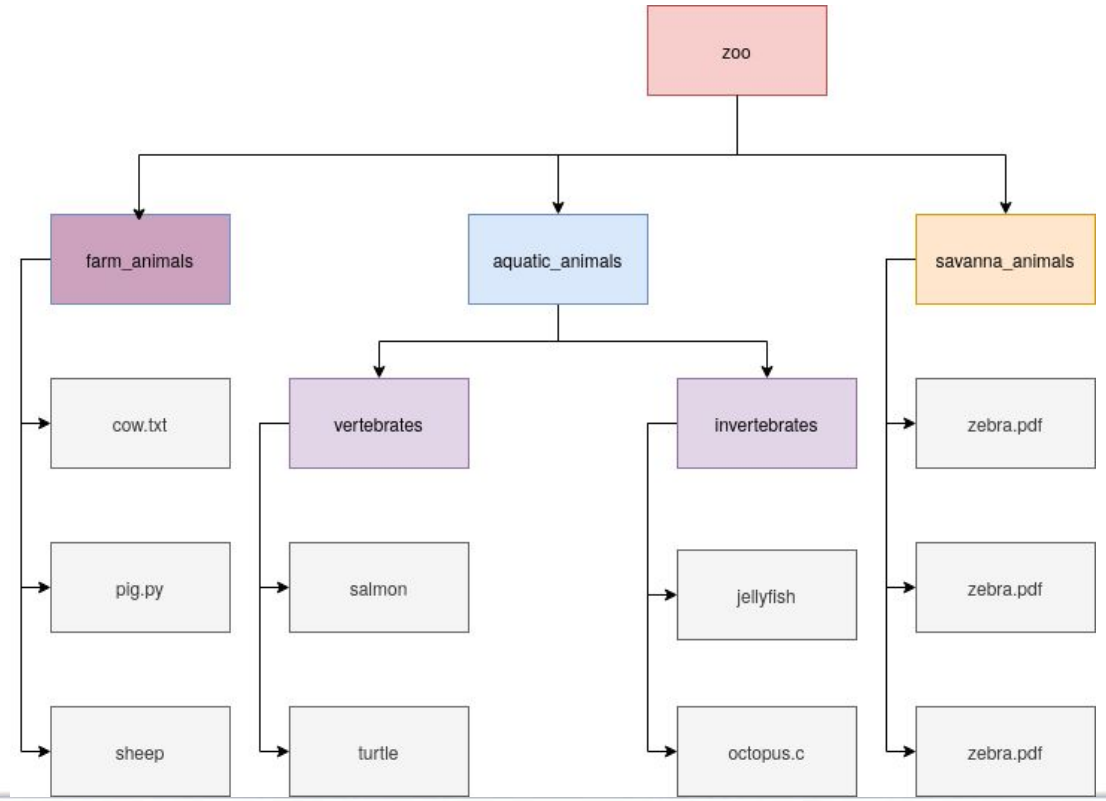
Solución



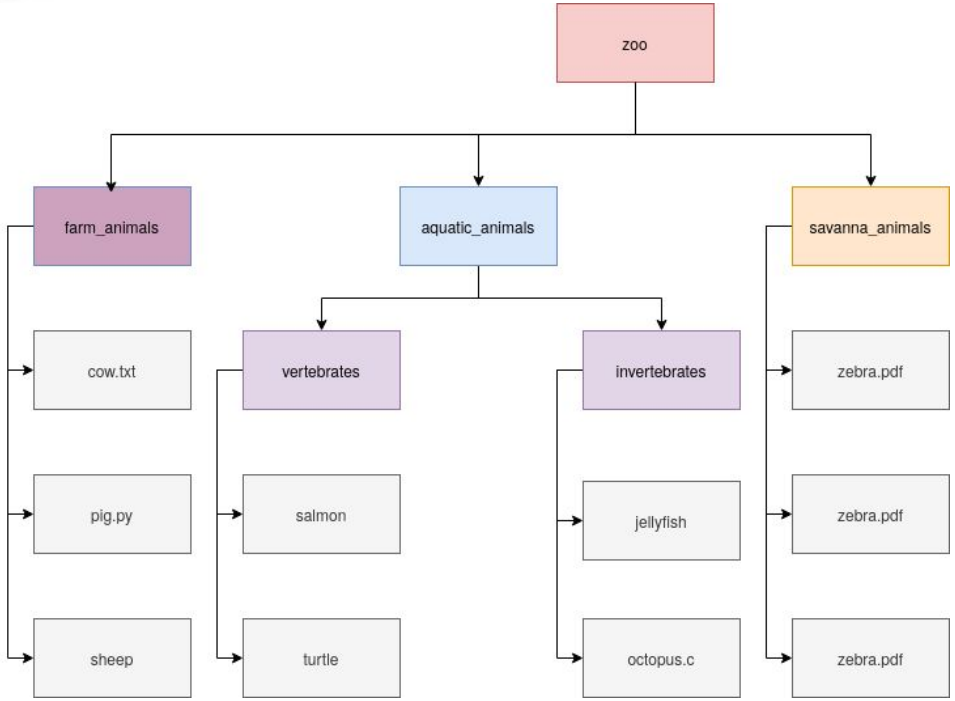

```
(base) omar@ubuntu:~/Documents/presentation/zoo$ cp aquatic_animals/invertebrates/turtle aquatic_animals/vertebrates/
(base) omar@ubuntu:~/Documents/presentation/zoo$ rm aquatic_animals/invertebrates/turtle
(base) omar@ubuntu:~/Documents/presentation/zoo$ ls aquatic_animals/vertebrates/
salmon  turtle
(base) omar@ubuntu:~/Documents/presentation/zoo$ ls aquatic_animals/invertebrates/
jellyfish  octopus.c
```

Ejercicio

Elimina el directorio forest_animals y lista los contenidos del directorio zoo en forma jerárquica o de árbol.



Solución




```
(base) omar@ubuntu:~/Documents/presentation/zoo$ rm -r forest_animals/
(base) omar@ubuntu:~/Documents/presentation/zoo$ tree
.
├── aquatic_animals
│   ├── invertebrates
│   │   ├── jellyfish
│   │   └── octopus.c
│   └── vertebrates
│       ├── salmon
│       └── turtle
├── farm_animals
│   ├── cow.txt
│   ├── pig.py
│   └── sheep
└── savanna_animals
    ├── deer.bak
    ├── giraffe
    └── lion.sh

6 directories, 10 files
```

Error común

No todas las distribuciones de Linux vienen con el comando ‘tree’ preinstalado, en caso de enfrentarse a esa situación se deberá instalar vía el administrador de paquetes predeterminado de la distribución a usar.

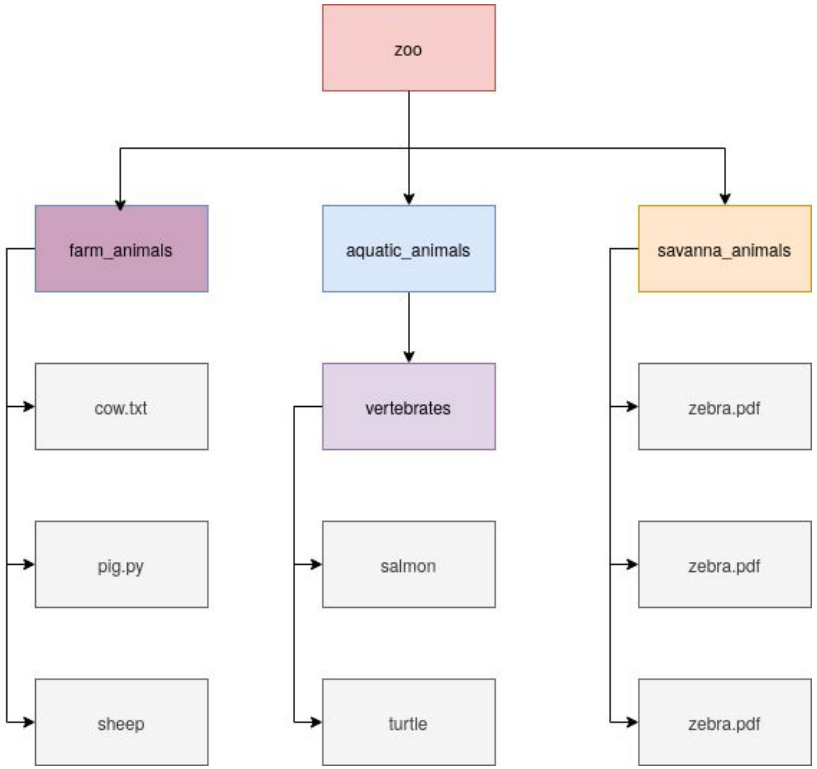
```
(base) omar@ubuntu:~/Documents/presentation/zoo$ tree
Command 'tree' not found, but can be installed with:
sudo snap install tree  # version 2.1.3+pkg-5852, or
sudo apt  install tree  # version 2.1.1-2
See 'snap info tree' for additional versions.
(base) omar@ubuntu:~/Documents/presentation/zoo$ sudo apt install tree
[sudo] password for omar:
Reading package lists... Done
Building dependency tree... Done
Reading state information... Done
The following NEW packages will be installed:
  tree
0 upgraded, 1 newly installed, 0 to remove and 20 not upgraded.
Need to get 47.1 kB of archives.
After this operation, 111 kB of additional disk space will be used.
Get:1 http://mx.archive.ubuntu.com/ubuntu noble/universe amd64 tree amd64 2.1.1-2ubuntu3 [47.1 kB]
Fetched 47.1 kB in 1s (79.2 kB/s)
Selecting previously unselected package tree.
(Reading database ... 163656 files and directories currently installed.)
Preparing to unpack .../tree_2.1.1-2ubuntu3_amd64.deb ...
Unpacking tree (2.1.1-2ubuntu3) ...
Setting up tree (2.1.1-2ubuntu3) ...
Processing triggers for man-db (2.12.0-4build2) ...
```

```
(base) omar@ubuntu:~/Documents/presentation/zoo$ tree .
.
├── acuatic_animals
│   ├── invertebrates
│   │   ├── jellyfish
│   │   └── octopus.c
│   └── vertebrates
│       ├── salmon
│       └── turtle
├── farm_animals
│   ├── cow.txt
│   ├── pig.py
│   └── sheep
└── savanna_animals
    ├── deer.bak
    ├── giraffe
    └── lion.sh

6 directories, 10 files
```

Ejercicio

Elimina el todos los archivos dentro del directorio aquatic_animals/invertebrates y posteriormente elimina el propio directorio vacío.



Solución

```
(base) omar@ubuntu:~/Documents/presentation/zoo$ rm aquatic_animals/invertebrates/*
(base) omar@ubuntu:~/Documents/presentation/zoo$ tree
.
├── aquatic_animals
│   ├── invertebrates
│   └── vertebrates
│       ├── salmon
│       └── turtle
├── farm_animals
│   ├── cow.txt
│   ├── pig.py
│   └── sheep
└── savanna_animals
    ├── deer.bak
    ├── giraffe
    └── lion.sh

6 directories, 8 files
(base) omar@ubuntu:~/Documents/presentation/zoo$ rmdir aquatic_animals/invertebrates/
(base) omar@ubuntu:~/Documents/presentation/zoo$ tree
.
├── aquatic_animals
│   └── vertebrates
│       ├── salmon
│       └── turtle
├── farm_animals
│   ├── cow.txt
│   ├── pig.py
│   └── sheep
└── savanna_animals
    ├── deer.bak
    ├── giraffe
    └── lion.sh

5 directories, 8 files
```

Ejercicios extras

Básico

https://linuxsurvival.com/

Intermedio

https://cmdchallenge.com

Comando	Descripción
echo “...” ‘... ‘ ´…´	imprimir texto
cat	muestra el contenido completo de archivos
>	Crear un archivo
>>	Agrupa (concatena) contenido
|	pipes
hostname	
lscpi lscpu	
vi	Editor de texto
nano	Editor de texto
emacs	Editor de texto (cargar modulo)

Componentes Básicos de un Script SLURM

Componentes Básicos de un Script SLURM

#!/bin/sh: Shell utilizado para ejecutar el script.

#SBATCH -p q1: Selección de la partición (cola) para el trabajo.

#SBATCH -n 1: Número de tareas solicitadas (en este caso, 1).

#SBATCH --time=hh:mm: Tiempo máximo de ejecución.

#SBATCH -o salida.txt : Salida o impresiones

#SBATCH -e error.txt : Errores o warning

Trabajos en Slurm

Crear el script SLURM: $ nano preba.slurm

```
#!/bin/sh
#SBATCH -p q1              # Nombre de la partición
#SBATCH -J Hostname        # Nombre del trabajo
#SBATCH -n 1               # Numero de nucleos (cores)
#SBATCH -o salida%j.txt    # Salida o impresiones
#SBATCH -e error%j.txt     # Errores o warning
sleep 5
hostname
```

Enviar el trabajo con: $ sbatch prueba.slurm

```
[crojas@chn02 ~]$ sbatch prueba.slurm
Submitted batch job 428043
```

Ejercicio 1

1: Crear un script: llamando run.sh

```
#!/bin/sh
#SBATCH -p q1
#SBATCH -n 1
hostname > file1.txt
```

2: leer el archivo run.sh

3: Ejecutar script: sbatch run.sh

4: leer el archivo: file1.txt

Hint:

- echo "..." >> run.sh
- nano run.sh
- vi run.sh
- Emacs run.sh

5: Modificar script anterior:

```
#!/bin/sh
#SBATCH -p q1
#SBATCH -n 2
hostname >> file2.txt
```

6: Ejecutar script: sbatch run.sh

7: Leer archivo de salida: file2.txt

Ejercicio 2
Script: run.sh

```
 GNU nano 2.9.8                                    run.sh

#!/bin/sh

#SBATCH -p q1                                  # Nombre de la partición
#SBATCH -J randomNum                           # Nombre del trabajo
#SBATCH -n 1                                   # Número de núcleos (cores)
#SBATCH -o salida.txt                         # Salida o impresiones
#SBATCH -e error.txt                          # Errores o warning

Error 2
echo "Esto se va a la salida estándar '-o'"
sleep 3

echo $RANDOM > numeroAlatorio.txt
echo hostname >> numeroAlatorio.txt
```

Solucion: ejercicio 1
Script: run.sh

1. `$ sbatch run.sh`
2. `$ ls`
3. `$ cat numeroAlatorio.txt`
4. `$ cat error.txt`
5. `$ cat salida.txt`
6. Edita run.sh y corrige el error y cambia la salida

```
$ cat error.txt
$ head error.txt
$ tail  error.txt
```

- https://shop.elsevier.com/books/high-performance-computing/sterling/978-0-12-420158-3
- https://www.ibm.com/topics/hpc
- https://insidehpc.com/hpc-basic-training/what-is-hpc/
- https://hbctraining.github.io/Intro-to-shell-fasrc-flipped/lessons/08_HPC_intro_and_terms.html