AGENT Portable Data Analysis Pipeline installation manual

Training of trainers to enable local dissemination of knowledge IPK Gatersleben 07 - 08 March 2023

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Introduction

This document is the installation manual for the AGENT Portable Data Analysis Pipeline, a readypackaged tool pipeline to support the analysis of large-scale genotyping data, with a particular focus on the genomics of genebanks. It has been developed as part of the AGENT project (http://www.agent-project.eu). This Manual describes the necessary setup to enable its use under Windows, macOS, and LINUX.

Use

The PDAP can be downloaded from Fairdom: <u>https://urgi.versailles.inrae.fr/fairdom/models/2</u> Once you have installed the software, please see the user guide (<u>https://urgi.versailles.inrae.fr/fairdom/documents/70</u>).

Test data Train the Trainer course

All the data needed for the hands on workshop can be downloaded here: <u>https://urgi.versailles.inrae.fr/fairdom/assays/109</u>

Prepare working directive

Download the singularity container and the Train the Trainer data and but them (option 1) in a Windows folder which can be accessed in the Ubuntu terminal by entering:

- "cd /mnt/c/..." for a folder on your C drive
- "cd /mnt/d/..." for a folder on your D drive

Or on your Ubuntu distribution (option 2)

• "explorer. exe ." to open the Windows-Explorer in the current directory of the Linux-filesystem

Installation

PDAP has been implemented to run in the <u>Singularity</u> platform. The Singularity platform runs natively in Linux; to deploy PDAP on the Windows or Mac operating systems, it is necessary to first install Windows Subsystem Linux (WSL) or a virtual machine.

Installation of WSL on windows 10/11

An option for running Singularity containers on Windows is to use Windows Subsystem for Linux (WSL2). However a Linux distribution needs to be installed like Ubuntu 20.04. This can be done through the Microsoft store (see Figure 1) or by the command terminal in windows with the command.

Code block 1: bash code to view available Linux distributions and install Ubuntu-20.04.

wsl –install

wsl --install Ubuntu-20.04



Installation Singularity on windows 10/11 using WSL

When the Ubuntu app is opened for the first time the user will be asked to set his/her username and create a user and set his/her sudo password (see Figure 2).



Figure 2. Set username and sudo password

Install system dependencies for Singularity by running the bash code of code block 2 in the Ubuntu terminal. When asked for your sudo password use the one set in Figure 2.

Code block 2: Update installed packages and install necessary packages. sudo apt-get update

```
sudo apt-get install -y build-essential libssl-dev uuid-dev libgpgme11-dev squashfs-
tools libseccomp-dev pkg-config
```

Use the bash code in code block 3 to download and install Singularity on your Ubuntu Linux distribution.

Code block 3: Download the Singularity installation package and install Singularity on WSL.

wget https://github.com/sylabs/singularity/releases/download/v3.9.7/singularityce_3.9.7-focal_amd64.deb

sudo apt install ./singularity-ce_3.9.7-focal_amd64.deb

Installation on Windows 10/11 or macOS using Vagrant Virtual Machine Install Oracle VirtualBox, install Vagrant, and install Vagrant-manager and Git for windows. More information can be found here: <u>https://sylabs.io/guides/3.5/admin-guide/installation.html#installation-on-windows-or-mac</u>

Download and install Git.

- Windows: <u>https://gitforwindows.org/</u>
- macOS: <u>https://git-scm.com/download/mac</u>

Open the Git Bash terminal and create and enter a directory which will be used with your Vagrant VM (code block 4).

```
Code block 4: Create and enter a Vagrant virtual machine directory.
mkdir vm-singularity
```

Issue the commands from code block 5 step by step to bring up the Virtual Machine.

Code block 5: Start a virtual machine with singularity installed export VM=sylabs/singularity-3.5-ubuntu-bionic64 vagrant init \$VM vagrant up vagrant ssh, this will make a connection to your VM.

Check the version of singularity (and that it has installed correctly) using the command "singularity --version".

Installation on Linux (Ubuntu)

Please install the Singularity package, if it is not already installed with commands from **code block 3**. More information can be found here: <u>https://sylabs.io/guides/3.5/admin-guide/installation.html#installation-on-linux</u>

Appendix 1: Activate virtualization in BIOS

Tested with Windows 10 Enterprise LTSC 2019 (1809) and Ubuntu 20.04 LTS

Step 1: Activate Virtualization in BIOS

Example Asus BIOS			
ASUS UEFI BIOS Utility – Advanced Mode			
11/28/2017 13:48 🌣 🌐 English 🖆 MyFavorite(F3) 🏷 Qfan Control(F6) 🖓 EZ Tuning Wizard(F11) 통 Quick Note(F3	9) ? Hot Keys		
My Favorites Main Ai Tweaker <u>Advanced</u> Monitor Boot Tool Exit	Hardware Monitor		
L3 Cache 6 MB	CPU		
L4 Cache Not Supported	Frequency Temperature		
Intel Adaptive Thermal Monitor	3500 MHz 27°C		
Active Processor Cores	BCLK Vcore 100.0 MHz 1.024 V		
Limit CPUID Maximum Disabled -			
Execute Disable Bit	35x		
Intel Virtualization Technology	Memory		
Hardware Prefetcher(L2 Cache)	Frequency Voltage 1600 MHz 1.500 V		
Adjacent Cache Line Prefetcher Enabled -	Capacity 8102 MB		
Boot performance mode Max Non-Turbo Performance 👻			
Dynamic Storage Accelerator Disabled -	Voltage		
➤ CPU Power Management Configuration	+12V +5V 12.000 V 5.080 V		
Intel Virtualization Technology makes a single system appear as multiple independent systems to software. This allows for multiple, independent operating systems to be running simultaneously on a single system.	+3.3V 3.328 V		
Last M	lodified EzMode(F7)		
Version 2.16.1240. Copyright (C) 2015 American Megatrends, Inc.			

Appendix 2: Activate optional feature "Windows-Subsystem for Linux"

Choose Option 1 OR Option 2

OPTION 1: Activate Feature through Windows Settings

1. Navigate to Control Panel>Programs>activate or deactivate Windows-Features



2. Tick the box "Windows-Subsystem for Linux" and press "OK"

💽 Windows-Features	—		×
Windows-Features aktivieren oder de	aktivi	eren	?
Verwenden Sie die Kontrollkästchen, um die entsp oder auszuschalten. Ein ausgefülltes Kontrollkäste Feature nur teilweise aktiviert ist.	rechen hen be	den Feature deutet, dass	es ein- s ein
Windows Defender Application Guard			^
Windows Hypervisor Platform			
Windows Identity Foundation 3.5			
🕀 🔽 🔜 Windows PowerShell 2.0			
Windows Projected File System			
Windows TIFF IFilter			
🗄 🔲 🔛 Windows-Prozessaktivierungsdienst			
🗹 🔄 Windows-Subsystem für Linux			
Work Folders Client			
			~
<			>
ОК		Abbrech	ien

3. Press "Restart now" and continue with "Step 3: Install Ubuntu distribution"



OPTION 2:

Activate Feature through PowerShell-Script

- Open a Windows PowerShell prompt AS ADMINISTRATOR
- Execute the command in code block 6.

Code block 6.

Enable-WindowsOptionalFeature -Online -FeatureName Microsoft-Windows-Subsystem-Linux

• Restart your PC

Appendix 3: Installing WSL manually (without Windows Store)

Step 1: Install Ubuntu distribution

• Open a Windows PowerShell prompt (<u>NOT</u> AS ADMINISTRATOR) Execute the following commands in code block 7

Code block 7.

Invoke-WebRequest -Uri https://aka.ms/wslubuntu2004 -OutFile Ubuntu.appx -UseBasicParsing

Add-AppxPackage .\Ubuntu.appx

Hint:

Newer Windows Versions supports Ubuntu 22.04 LTS Invoke-WebRequest -Uri https://aka.ms/wslubuntu2204 -OutFile Ubuntu.appx -UseBasicParsing

Step 2: Create Linux user and password

1. Open Ubuntu through the Start Menu



2. Ubuntu will start installing, this may take a while

🧿 Ubuntu	-	\times
Installing, this may take a few minutes		^

3. You are now prompted to create a username and password, choose any username and password you would like. This will be the root-account in the WSL



- 4. If everything is successful your Linux-terminal will look somewhat like this:
- 5. As a final step we recommend running "sudo apt update" and "sudo apt upgrade" to make sure that your environment is ready for use.

	—	\times
Installing, this may take a few minutes Please create a default UNIX user account. The username does not need to match your Windows username. For more information visit: https://aka.ms/wslusers Enter new UNIX username: schulung New password: Retype new password: passwd: password updated successfully Installation successful! To run a command as administrator (user "root"), use "sudo <command/> ". See "man sudo_root" for details.		^
Welcome to Ubuntu 20.04.3 LTS (GNU/Linux 4.4.0-17763-Microsoft x86_64)		
<pre>* Documentation: https://help.ubuntu.com * Management: https://landscape.canonical.com * Support: https://ubuntu.com/advantage System information as of Wed Feb 22 13:56:34 STD 2023 System load: 0.52 Users logged in: 0 Usage of /home: unknown IPv4 address for eth0: 10.10.17.23 Memory usage: 14% IPv4 address for eth1: 192.168.5.1</pre>		
Swap usage: 0% IPv4 address for eth2: 192.168.126.1 Processes: 7		
1 update can be applied immediately. To see these additional updates run: apt listupgradable		
The list of available updates is more than a week old. To check for new updates run: sudo apt update		
This message is shown once a day. To disable it please create the /home/schulung/.hushlogin file. schulung@bit-23:~\$		

Step 3: Find Linux user directory in Windows-Explorer

- 1. For moving files between your Windows environment and your Linux-environment you may want to know where your Linux filesystem is located in your Windows-filesystem
- 2. If you installed Ubuntu using the Windows Store, simply run "explorer. exe ." (note the extra .) from the WSL-terminal, this should open the Windows-Explorer in the current directory of the Linux-filesystem.
- 3. If you installed Ubuntu using the Powershell-Script from this guide or if the above command is not working for you, open up a PowerShell-prompt and type following command:

(Get-ChildItem HKCU:\Software\Microsoft\Windows\CurrentVersion\Lxss | ForEach-Object {Get-ItemProperty \$.PSPath}) | select DistributionName, @{n="Path";e={\$.BasePath + "\rootfs"}}