***Octopus for CentOS8***

# 在WSL ubuntu可直接安装

<https://octopus-code.org/documentation/13/ma>

nual/installation/windows\_build/

Building Octopus on Windows

Install of Octopus on Windows

In the following we look at how to install Octopus on a Windows, using Windows Subsystem for Linux (WSL). In the following, we assume that WSL2 is already installed. Else, run as administrator in PowerShell of Command prompt the command

wsl --install

Note that these instruction follow closely any Linux installation, so please refer to the linux installation for more advance options

Basic installation

In order to install Octopus, one needs first to install its dependencies. For a basic installation (without external libraries, no MPI nor GPU), please run first the following commands:

sudo apt install autoconf

sudo apt install libtool libtool-bin

sudo apt install g++

sudo apt install gfortran

sudo apt install make

sudo apt install libxc-dev

sudo apt install libfftw3-dev

sudo apt install libgsl-dev

sudo apt install libopenblas-dev

Then one can download Octopus (here Octopus 13.0 )

wget https://octopus-code.org/download/13.0/octopus-13.0.tar.gz

tar -xvf octopus-13.0.tar.gz

cd octopus-13.0

and configure it and install it as usual

./configure

sudo make install

As usual, a prefix could also be used to select the installation directory and “make check” can be used to check the correctness of the installation.

# CentOS-8

依赖库遇到困难依赖库名字改变

# 尝试采用Docker容器法

yum install -y yum-utils

yum-config-manager --add-repo https://download.docker.com/linux/centos/docker-ce.repo

yum install docker-ce docker-ce-cli containerd.io docker-buildx-plugin docker-compose-plugin

在安装 Docker 时遇到依赖问题，podman 和 buildah 这两个包存在冲突。它们都涉及容器技术，存在版本冲突。

删除冲突的软件包：

yum remove podman buildah

重新安装 Docker：

yum install -y docker-ce docker-ce-cli

yum install containerd.io

yum install -y docker-buildx-plugin docker-compose-plugin

# 启动docker

systemctl start docker

docker run hello-world

# 正式安装octopus

docker pull fangohr/octopus:12.1

# test if success. octopus version is displayed.

docker run --rm fangohr/octopus:12.1 octopus --version

# There are some trivial simulation configurations available in /opt/octopus-examples.

docker run --rm -ti -v $PWD:/io fangohr/octopus:12.1 bash

# cd one dir with inp, to start the octopus:

docker run --rm -ti -v $PWD:/io fangohr/octopus:12.1 octopus

# 退出伪终端TTY， exit 或 Ctrl + D

终止所有容器docker stop

使用 docker ps 查看运行容器ID

docker stop <容器ID或名称> 命令停止特定容器

# 复制文件到本地

打开另一个终端窗口，docker ps查找容器 ID。

docker cp CONTAINER\_ID:/io/example\_file.txt /path/on/local/system/

从 Docker 容器中将文件复制到本地系统。