



udocker - *be anywhere*

Part 3 - Hands On: intermediate stuff

<https://github.com/indigo-dc/udocker>

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Recap from last slide deck: udocker

Installation

- The end user can download and execute `udocker` without system administrator intervention.
- Install from a released version:
 - Download a release tarball from <https://github.com/indigo-dc/udocker/releases>:

```
wget https://github.com/indigo-dc/udocker/releases/download/1.3.17/udocker-1.3.17.tar.gz
tar zxvf udocker-1.3.17.tar.gz
export PATH=`pwd`/udocker-1.3.17/udocker:$PATH
udocker install
```

Importing and exporting, loading and saving: images and containers

I have a dockerfile!

- But `udocker` does not support `build` the dockerfile...
 - Use `docker` itself in you <lap|desk>top
 - Example: <https://github.com/mariojmdavid/docker-gromacs-cuda/blob/master/gromacs-cpu/Dockerfile-cpu>

```
git clone https://github.com/mariojmdavid/docker-gromacs-cuda.git
cd docker-gromacs-cuda/gromacs/
docker build --build-arg gromacs_ver=2025.4 -t gromacs-openmp-2005.4 -f Dockerfile-cpu .

## Or you can build instead the GPU version
docker build --build-arg gromacs_ver=2025.4 -t gromacs-gpu-2005.4 -f Dockerfile-gpu .
```

- (Will take quite awhile, 30 minutes on my desktop)

I have a docker image!

After you build the image with docker:

```
docker images
```

REPOSITORY	TAG	IMAGE ID	CREATED	SIZE
gromacs-openmp-2005.4	latest	e0228510f76f	22 minutes ago	456MB

Save the image with `docker` to a tarball:

```
docker save -o gromacs.tar gromacs-openmp-2005.4
```

udocker load

You can load a tarball with `udocker` that is a docker image, and that you saved previously with docker:

```
udocker load -i gromacs.tar gromacs-omp-2005.4
```

And now you can check several things:

```
udocker images  
REPOSITORY  
gromacs-omp-2005.4:latest
```

Create a container and run it

```
udocker create --name=grom gromacs-openmp-2005.4
```

```
udocker ps
```

CONTAINER ID	P	M	NAMES	IMAGE
e2e014d9-9770-3fb5-a4a9-098a95371adf	.	W	['grom']	gromacs-openmp-2005.4:latest

```
udocker run grom env
```

```
*****
*
*          STARTING e2e014d9-9770-3fb5-a4a9-098a95371adf
*
*****
executing: env
PATH=/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin:/usr/local/gromacs/bin
LD_LIBRARY_PATH=/usr/local/gromacs/lib
```

Running gromacs with **udocker**

```
udocker run grom gmx mdrun -h
```

```
*****
*
*          STARTING ad754a36-b951-38da-a116-a05fb572d7ca
*
*****
```

```
executing: gmx
```

```
:-) GROMACS - gmx mdrun, 2025.4 (-:
```

```
Executable:  /usr/local/gromacs/bin/gmx
```

```
Data prefix: /usr/local/gromacs
```

```
Working dir: /home
```

```
Command line:
```

```
gmx mdrun -h
```

```
SYNOPSIS
```

```
gmx mdrun [-s [<.tpr>]] [-cpi [<.cpt>]] [-table [<.xvg>]] [-tablep [<.xvg>]]
```

```
...
```


Environment in dockerfile is preserved - I

You can check the dockerfile: <https://github.com/mariojmdavid/docker-gromacs-cuda/blob/master/gromacs-cpu/Dockerfile-cpu>

```
FROM ubuntu:24.04
LABEL maintainer="Mario David <mariojmdavid@gmail.com>"
ARG gromacs_ver
RUN apt-get update \
...
ENV PATH=$PATH:/usr/local/gromacs/bin
ENV LD_LIBRARY_PATH=/usr/local/gromacs/lib
WORKDIR /home
```

Environment in dockerfile is preserved in **udocker** container - II

Just check the **ENV** and **WORKDIR**:

```
udocker run grom env
...
PATH=/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin:/usr/local/gromacs/bin
LD_LIBRARY_PATH=/usr/local/gromacs/lib

udocker run grom pwd
...
/home
```

I want to install/compile in a container! - I

Pull some base image, create a container and run:

```
udocker pull almalinux:9  
udocker create --name=mypython almalinux:9  
udocker run mypython bash
```

And after that install and/or compile whatever you want

I want to install/compile in a container! - II

Now you are inside the container and seems you are `root`:

```
dnf -y install python3 gcc-c++ python3-pip  
pip-3 install numpy matplotlib scipy  
exit
```

You are satisfied so, you exit the container, but... I want to preserve what I installed.

udocker export and import

You can export a container into a tarball, for safekeeping:

```
udocker export -o mypython.tar mypython
```

Now you can import this container into an image with a given tag (empty tag defaults to `latest`):

```
udocker import mypython.tar mypython:v1.0
```

udocker list images long format

```
udocker images -l  
REPOSITORY  
...  
almalinux:9 .  
  /home/david/.udocker/repos/almalinux/9  
    /sha256:c9bcec02f046478f7ecf78b9568b666cc3b63a2effe339b1022e3b550faca3e8 (0 MB)  
    /sha256:08d3c44badca17b0b810e53779272d43e9542081ae05f516071ae4d5d2369271 (67 MB)  
mypython:v1.0 .  
  /home/david/.udocker/repos/mypython/v1.0  
    /9e1605be9a6064f41fe0ee83c6ad3cd644d77d5b3c8ff45af4157719ccd627a3.json (0 MB)  
    /9e1605be9a6064f41fe0ee83c6ad3cd644d77d5b3c8ff45af4157719ccd627a3.layer (780 MB)
```

About mounting volumes and directories

Mounting a directory in the container - I

Assume you have a directory you want to use inside the container.

First grab yourself a tpr file:

```
mkdir -p $HOME/udocker-tutorial/gromacs/input  
cd $HOME/udocker-tutorial/gromacs/input/  
wget --no-check-certificate https://download.a.acnca.pt/webdav/gromacs-input/md.tpr
```


Mounting a directory in the container - II

We will bind mount the directory in the `/home/user` inside the container (if this directory does not exist inside the container, then it will be created):

```
udocker run -v=$HOME/udocker-tutorial/gromacs:/home/user -w=/home/user grom /bin/bash
```

Mounting a directory in the container - III

Now, inside the container:

```
ls -al
total 12
drwxrwxr-x 3 root root 4096 Apr  4 08:31 .
drwxr-xr-x 3 root root 4096 Apr  4 08:42 ..
drwxrwxr-x 2 root root 4096 Apr  4 08:31 input
```

Mounting a directory in the container - IV

Inside the container - make a directory for your output, and run your favourite molecular dynamics

simulation software, (if you want wait a few minutes to finish, will not take long):

```
mkdir output
cd output
gmx mdrun -s /home/user/input/md.tpr -deffnm ud-tutorial \
    -maxh 0.50 -rethway -noconfout -nstps 10000 -g logfile

exit
```

Mounting a directory in the container - V

And back to your preferred machine:

```
ls $HOME/udocker-tutorial/gromacs/output  
logfile.log  ud-tutorial.edr  ud-tutorial.trr  ud-tutorial.xtc
```

All nice output files right there in you home directory.

End of Hands On part II

