

CellOrganizer Installation Instructions



To chat with the team use the #cellorganizer channel in Slack

[CLICK HERE TO CHAT WITH US](#)

Required OS/Hardware

1. MacOSX High Sierra or newer
2. Linux, Debian 8, 9, 10, CentOS 7
3. Windows 10
4. At least 15Gb of free space for the container and the datasets we will be using.

If you are not sure you have the right hardware, feel free to ask us.

Required Software

Docker



Docker is necessary for the tutorials on the afternoon of Day 3 and the advanced topics session on Day 4.

In order to download the image we will be using for the workshop you will need to install Docker. To install Docker follow the instructions [here](#).

If have any questions regarding installing Docker, feel free to message the team on Slack in the #cellorganizer channel.

About Docker

- A Docker image is a file, composed of multiple layers, that is used to execute code in a Docker container. When we run the `docker pull` command we are going to be downloading the CellOrganizer for Docker image from [Docker Hub](#).
- A container is a standard unit of software that packages code and all its dependencies.
- Docker images become containers at runtime. When we execute the `docker run` command we start a container.

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- In Linux, the Docker daemon starts when you boot your machine, but in MacOSX and Windows we need to manually start it.
- In MacOSX you should be able to find the application using Spotlight



- It is similar in Windows, just search for Docker.
- If you see this message when you try to run any Docker command it means that Docker has not started or has crashed.

```
icaoberg@MacBook-Pro: ~  
→ ~ docker ps  
Cannot connect to the Docker daemon at unix:///var/run/docker.sock. Is the docker daemon running?  
→ ~
```

- If you would like to test if Docker is working properly you can run the command `docker pull ubuntu`, to pull an Ubuntu Docker image

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```
icaoberg@MacBook-Pro: ~  
→ ~ docker pull ubuntu  
Using default tag: latest  
latest: Pulling from library/ubuntu  
a4a2a29f9ba4: Pull complete  
127c9761dcba: Pull complete  
d13bf203e905: Pull complete  
4039240d2e0b: Pull complete  
Digest: sha256:35c4a2c15539c6c1e4e5fa4e554dac323ad0107d8eb5c582d6ff386b383b7dce  
Status: Downloaded newer image for ubuntu:latest  
docker.io/library/ubuntu:latest  
→ ~
```

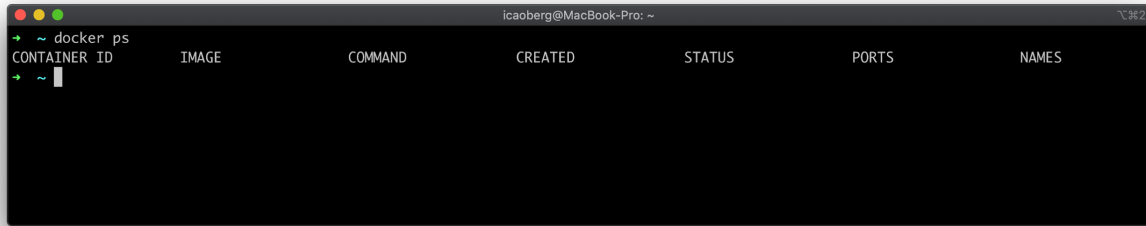
- To list the Docker images in your system, run the `docker images` command

```
icaoberg@MacBook-Pro: ~  
→ ~ docker images  
REPOSITORY          TAG                 IMAGE ID            CREATED             SIZE  
ubuntu               latest             74435f89ab78       3 days ago         73.9MB  
→ ~
```

- To delete the image from your system, run the `docker rmi <IMAGE ID>` command

```
icaoberg@MacBook-Pro: ~  
→ ~ docker rmi 74435f89ab78  
Untagged: ubuntu:latest  
Untagged: ubuntu@sha256:35c4a2c15539c6c1e4e5fa4e554dac323ad0107d8eb5c582d6ff386b383b7dce  
Deleted: sha256:74435f89ab7825e19cf8c92c7b5c5ebd73ae2d0a2be16f49b3fb81c9062ab303  
Deleted: sha256:8a8d1f0b34041a66f09e49bdc03e75c2190f606b0db7e08b75eb6747f7b49e11  
Deleted: sha256:f1b8f74eff975ae600be0345aaac8f0a3d16680c2531ffc72f77c5e17cbfeeee  
Deleted: sha256:27d46ebb54384edbc8c807984f9eb065321912422b0e6c49d6a9cd8c8b7d8ffc  
Deleted: sha256:e1c75a5e0bfa094c407e411eb6cc8a159ee8b060cbd0398f1693978b4af9af10  
→ ~
```

- To list all the running Docker containers, run the command `docker ps` command



```
icaoberg@MacBook-Pro: ~  
➔ ~ docker ps  
CONTAINER ID    IMAGE    COMMAND    CREATED    STATUS    PORTS    NAMES
```

- This workshop is not about using Docker and the commands above should be all that you need to know. However [here](#) is a cheat sheet in case you would like to know more.

CellOrganizer for Jupyter



The Docker image is available to pull

<https://hub.docker.com/repository/docker/murphylab/cellorganizer-jupyter>

Just follow the instructions below

Summary

- You will pull (download) a Docker image from DockerHub to your laptop/desktop.
- You will create a folder on your desktop
- You will start a Docker instance from the Docker image you pulled and you will attach the local folder to your instance

CellOrganizer for Docker Instructions for MacOSX/Linux



See the instructions acted out on video

https://youtu.be/7_Yqr5zQ1tA

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Pulling the image

- Open a Terminal
- In terminal type the following command to create a folder in your desktop
 - `mkdir ~/Desktop/mmbios2021`
- In terminal type following command to pull the Docker image from DockerHub
 - `docker pull murphylab/cellorganizer-jupyter:mmbios2021`
- Running the command above should produce output like this.
- If you type the command `docker images` in terminal, then you should see the image you just pulled.

Starting a container

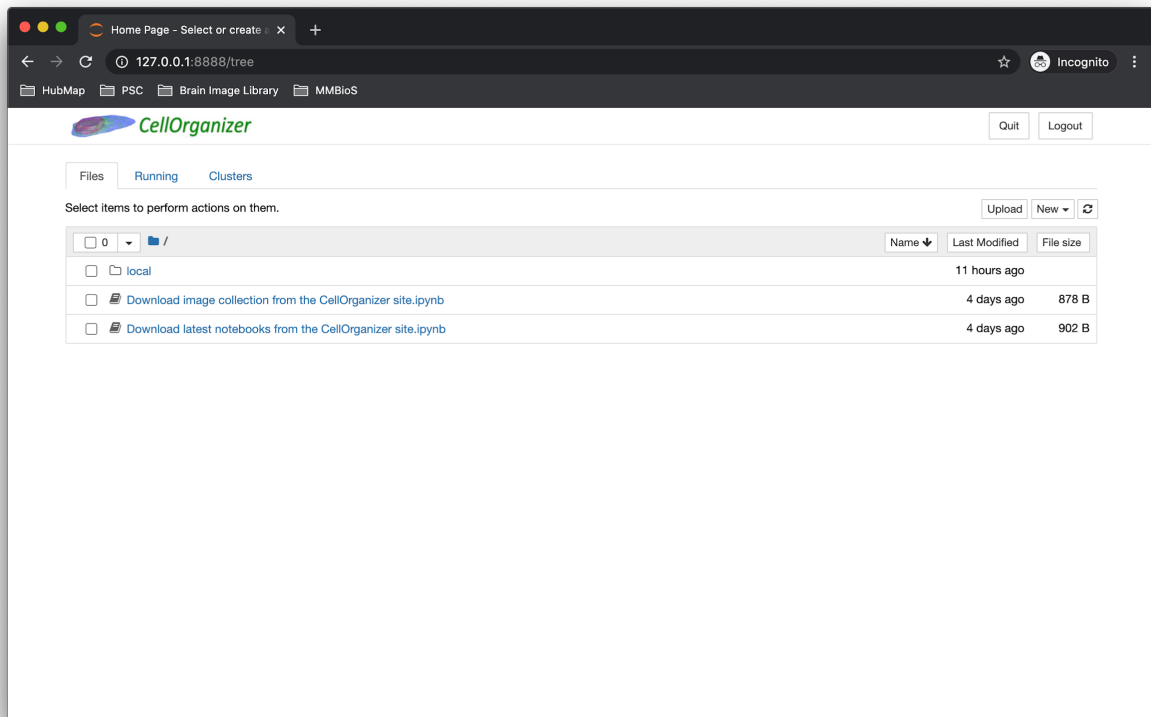
- To start the container type the command
 - In Linux type
 - `chmod a+rx -R ~/Desktop/mmbios2021/ && docker run --rm -p 8888:8888 -v ~/Desktop/mmbios2021:/home/murphylab/cellorganizer/local --memory="4g" --cpus=2 -e JUPYTER_LAB_ENABLE=yes murphylab/cellorganizer-jupyter:mmbios2021`
 - In MacOSX type
 - `docker run --rm -p 8888:8888 -v ~/Desktop/mmbios2021:/home/murphylab/cellorganizer/local --memory="4g" --cpus=2 -e JUPYTER_LAB_ENABLE=yes murphylab/cellorganizer-jupyter:mmbios2021`
- If the container started properly, then you should see a screen like this

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```
er
[I 06:52:57.765 NotebookApp] The Jupyter Notebook is running at:
[I 06:52:57.765 NotebookApp] http://7b40c5ca1902:8888/?token=3d1d74fcef0ff69b5097c9f85092f606ac9
94eee1587ec82
[I 06:52:57.765 NotebookApp] or http://127.0.0.1:8888/?token=3d1d74fcef0ff69b5097c9f85092f606ac
994eee1587ec82
[I 06:52:57.765 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice
to skip confirmation).
[C 06:52:57.768 NotebookApp]

To access the notebook, open this file in a browser:
file:///home/jovyan/.local/share/jupyter/runtime/nbserver-6-open.html
Or copy and paste one of these URLs:
http://7b40c5ca1902:8888/?token=3d1d74fcef0ff69b5097c9f85092f606ac994eee1587ec82
or http://127.0.0.1:8888/?token=3d1d74fcef0ff69b5097c9f85092f606ac994eee1587ec82
```

- The URL at the end of the message will be different for all of you, as the URL contains a token.
- Copy the URL and copy it in a web browser



- If you see a page like the image above, then you are ready to start using CellOrganizer.



- **Run the download notebook to pull models, notebooks and images needed for the demos and tutorial modules**
- To stop the Jupyter instance, go to Terminal and click `Control+c`.
- Since the containers have been saving your results to the local folder you created at the beginning, it means that stopping the Jupyter notebook does not erase the results you have computed so far.
- [Linux users will have to do this additional step.](#)

CellOrganizer for Docker Instructions for Windows

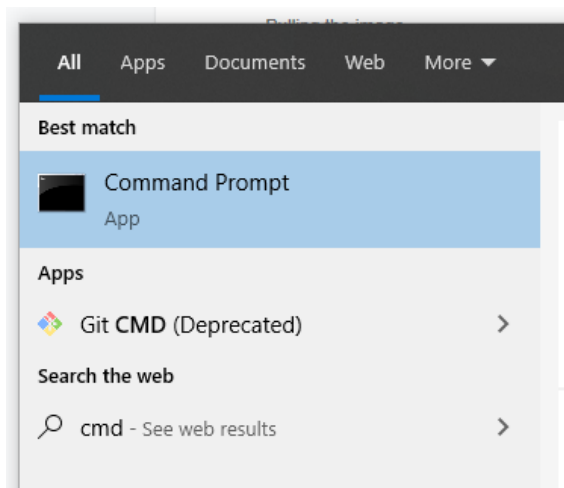


See the instructions acted out on video

https://youtu.be/HwvGKOs_Bbg

Pulling the image

- Open a Terminal



- In terminal type the following command to create a folder in your desktop (double quotes below are necessary if your username has whitespaces)
 - `mkdir "%userprofile%\Desktop\mmbios2021"`



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```
Command Prompt

C:\Users\Computational Bio>mkdir "%userprofile%\Desktop\mmbios2020"

C:\Users\Computational Bio>ls -lt "%userprofile%\Desktop"
total 17
drwxr-xr-x 1 Computational Bio 197121  0 Jun 24 01:01  mmbios2020
-rw-r--r-- 1 Computational Bio 197121 1084 Jun  3 18:18  script.sh
-rw-r--r-- 1 Computational Bio 197121  282 Jun  3 18:03  desktop.ini
-rwxr-xr-x 1 Computational Bio 197121 2144 Jun  3 17:57  'Docker Desktop.lnk'
-rwxr-xr-x 1 Computational Bio 197121 2418 Jun  3 16:46  'Microsoft Teams.lnk'
-rwxr-xr-x 1 Computational Bio 197121 1450 May 20 18:13  'Microsoft Edge.lnk'

C:\Users\Computational Bio>
```

- In terminal type following command to pull the Docker image from DockerHub
 - `docker pull murphylab/cellorganizer-jupyter:mmbios2021`
- If you type the command `docker images` in terminal, then you should see the image you just pulled.

```
Command Prompt

Status: Downloaded newer image for murphylab/cellorganizer-jupyter:mmbios2020
docker.io/murphylab/cellorganizer-jupyter:mmbios2020

C:\Users\Computational Bio>docker images
REPOSITORY          TAG                 IMAGE ID            CREATED             SIZE
murphylab/cellorganizer-jupyter  mmbios2020         6845f71b255a       6 hours ago        10GB

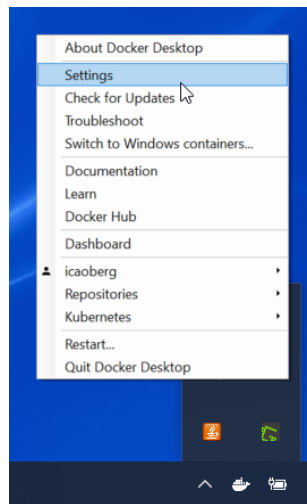
C:\Users\Computational Bio>
C:\Users\Computational Bio>
```

Making your local folder available to Docker

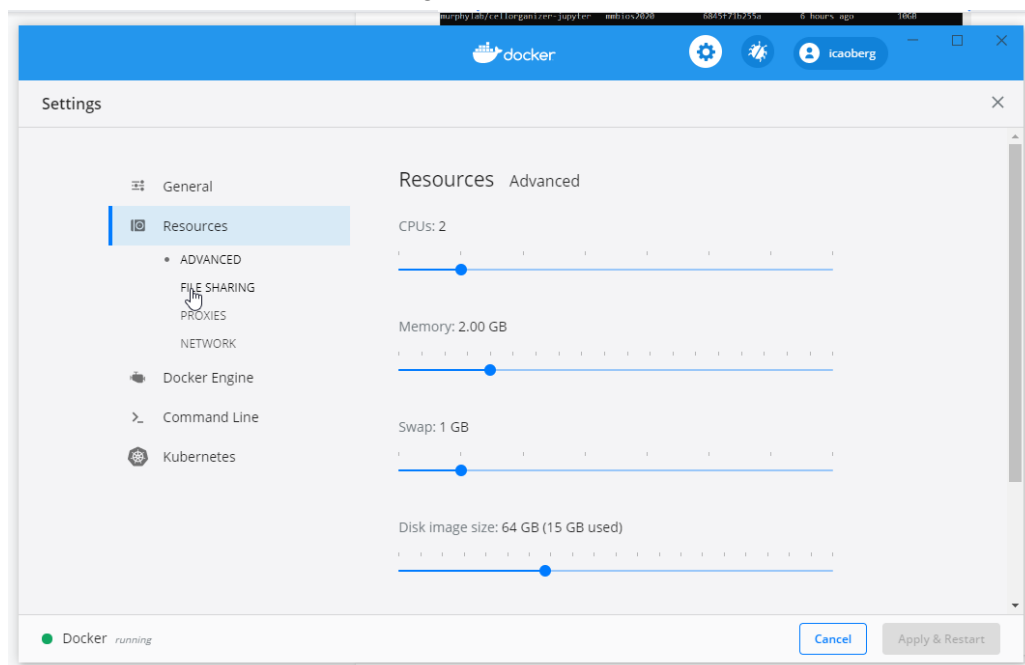
This is an extra step for Windows.

- Click on Docker settings

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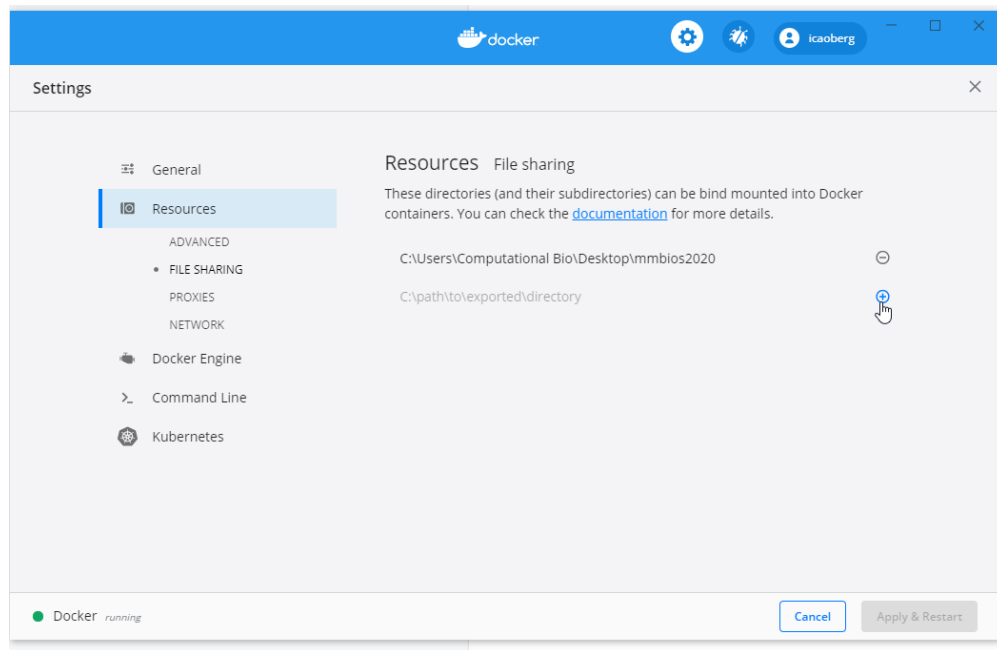


- Click on Resources > File Sharing



- And select the folder you created by clicking (+) and searching for the folder you created in your desktop

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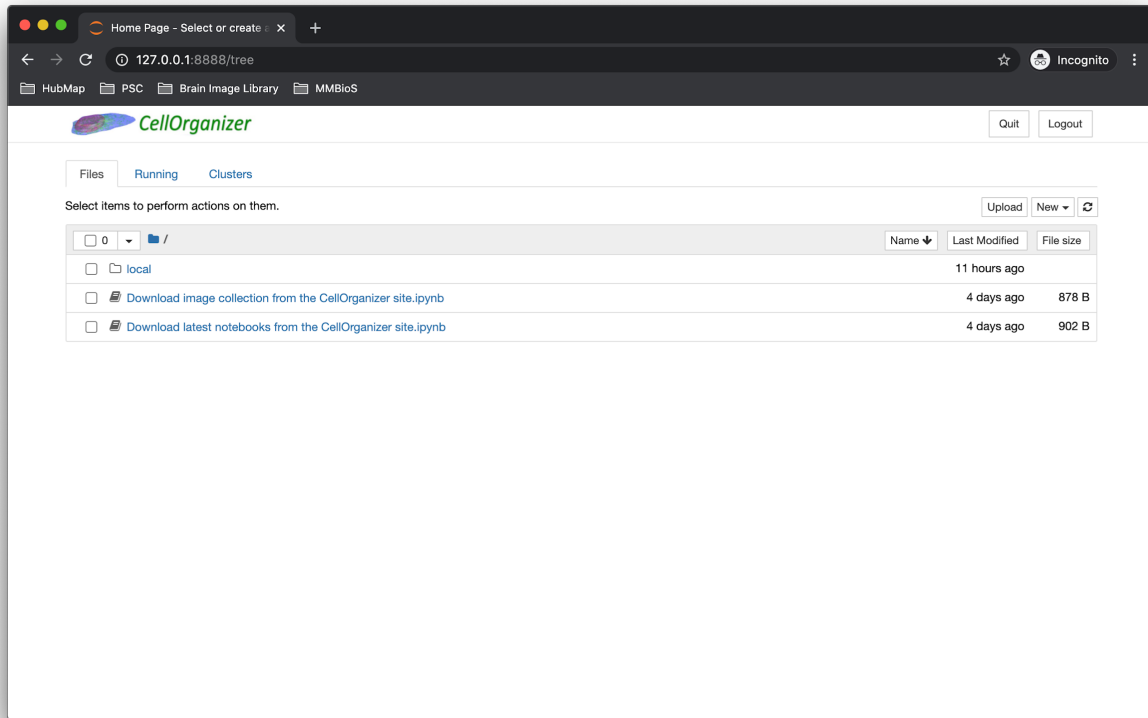


- Then click Apply and Restart. And wait.

Starting the container

- To start the container type the command
 - `docker run --rm -p 8888:8888 -v "%userprofile%\Desktop\mmbios2021:/home/murphylab/cellorganizer/local --memory="4g" --cpus=2 -e JUPYTER_LAB_ENABLE=yes murphylab/cellorganizer-jupyter:mmbios2021`
- If the container started properly, then you should see a screen like this
- The URL at the end of the message will be different for all of you, as the URL contains a token.
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VirtualCell



This software is needed for those interested in
Advanced Topic 4 - Simulating cell biochemistry with different geometries

VCell (Virtual Cell) is a comprehensive platform for modeling cell biological systems that is built on a central database and disseminated as a web application.

To download VirtualCell click [here](#).

Fiji



This software is needed for those interested in
Advanced Topic 5 - Working with your own images

[Fiji](#) is an image processing package—a "batteries-included" distribution of [ImageJ](#), bundling a lot of plugins which facilitate scientific image analysis.

To download Fiji click [here](#).