



“Containerization in HPC” course tutorial

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ABOUT THE TUTORIAL

In this tutorial, we provide the preliminary steps to attend the “Containerization in HPC” CINECA course. We list some ssh connection tools, mainly for Windows users. We explain the installation instructions for Singularity and Docker, since the build of containers will be done on your local workstation, while the run and execution will be done on GALILEO CINECA HPC cluster, the one chosen for the hands on of the course. Then, we provide the instructions to set up GitHub, Docker Hub and Singularity Hub, to simplify the sharing and the automated build containers process. We provide instructions for Linux users. The instruction links for Windows and Mac users are also listed.

We strongly recommend to install Singularity and Docker platforms and set up and sign up into the hubs before the beginning of the course.

If you meet troubles in the procedures explained, please contact us by sending an email to corsi.hpc@cineca.it before the beginning of the course.



SSH CONNECTION

In order to attend this course you will need to connect to GALILEO CINECA HPC cluster via secure shell (ssh).

If you are using Linux or MacOS, you already have the ssh command in the OS shell.

If you are using Windows, you can use ssh in PowerShell or in Command Prompt (cmd.exe). If you encounter trouble, we suggest (recommend) to install and use one of these three tools:

- 1) PuTTY - <https://www.putty.org/>
- 2) GitBash - <https://gitforwindows.org/>
- 3) Secure Shell extension for Chrome - <https://chrome.google.com/webstore/detail/secure-shell/iodihamcpbpeioa>
jjeobimgagajmlbd - You must open this link with Chrome or Chromium browser.

DOCKER INSTALLATION

Official reference link: <https://docs.docker.com/get-docker/>

Linux Users

Install Docker Engine on your Linux workstation.

A variety of Linux platforms are supported, like CentOS, Debian, Fedora, Raspbian and Ubuntu, please refer to <https://docs.docker.com/engine/install/> .

Hereafter the procedure for a CentOS7 is described, using the official .rpm packages provided by Docker.

Uninstall old versions of Docker, if present. Then open a shell in your workstation and run the following commands, to set up the repository and install Docker Engine:

```
$ sudo yum install -y yum-utils
$ sudo yum-config-manager --add-repo \
    https://download.docker.com/linux/centos/docker-ce.repo
$ sudo yum install docker-ce docker-ce-cli containerd.io
```



If every step was fine so far, congratulations: you have installed Docker on our workstation.

Now, start Docker and verify that it is installed correctly with the following commands:

```
$ sudo systemctl start docker
$ sudo docker run hello-world
```

The last command downloads a test image and runs it in a container. When the container runs, it prints an informational message and exits.

Now, to use Docker as a non-root user, you need to add your own user into the “docker” linux group:

```
$ sudo groupadd docker
$ sudo usermod -aG docker $USER
```

Log out and log back in so that your group membership is re-evaluated. Verify that you can run docker commands without sudo running:

```
$ docker run hello-world
```

If you have installed docker correctly on your workstation, the result should be:



```
[smarocchi@NSMAROCCH204664 ~]$ docker run hello-world
Unable to find image 'hello-world:latest' locally
latest: Pulling from library/hello-world
0e03bdcc26d7: Already exists
Digest: sha256:8c5aeeb6a5f3ba4883347d3747a7249f491766ca1caa47e5da5dfcf6b9b717c0
Status: Downloaded newer image for hello-world:latest

Hello from Docker!
This message shows that your installation appears to be working correctly.

To generate this message, Docker took the following steps:
1. The Docker client contacted the Docker daemon.
2. The Docker daemon pulled the "hello-world" image from the Docker Hub.
   (amd64)
3. The Docker daemon created a new container from that image which runs the
   executable that produces the output you are currently reading.
4. The Docker daemon streamed that output to the Docker client, which sent it
   to your terminal.

To try something more ambitious, you can run an Ubuntu container with:
$ docker run -it ubuntu bash

Share images, automate workflows, and more with a free Docker ID:
https://hub.docker.com/

For more examples and ideas, visit:
https://docs.docker.com/get-started/

[smarocchi@NSMAROCCH204664 ~]$
```

Windows or Mac Users

Please, for Windows refer to: <https://docs.docker.com/docker-for-windows/install/>

For Mac, refer to: <https://docs.docker.com/docker-for-mac/install/>

SINGULARITY INSTALLATION

Official reference link: <https://sylabs.io/guides/3.6/admin-guide/>

Linux Users

It is possible to install Singularity using the CentOS/RHEL .rpm package that is regularly updated into the EPEL (Extra Packages for Enterprise Linux) repos.

Open a shell and run the following commands to update your system and install the EPEL repo and Singularity:

```
$ sudo yum update -y && \
  sudo yum install -y epel-release && \
  sudo yum update -y && \
  sudo yum install -y singularity
```



If the previous solution does not work on your laptop, or for another Linux distribution, you can install Singularity from source.

Open a terminal, and install all the needed dependencies:

-- Red Hat Enterprise Linux or CentOS

```
$ sudo yum update -y && \  
    sudo yum groupinstall -y 'Development Tools' && \  
    sudo yum install -y \  
    openssl-devel \  
    libuuid-devel \  
    libseccomp-devel \  
    wget \  
    squashfs-tools \  
    cryptsetup
```

-- Ubuntu or Debian

```
$ sudo apt-get update && sudo apt-get install -y \  
    build-essential \  
    uuid-dev \  
    libgpgme-dev \  
    squashfs-tools \  
    libseccomp-dev \  
    wget \  
    pkg-config \  
    git \  
    cryptsetup-bin
```

Now, by root user, install Go with the following commands:

```
$ cd /tmp/  
$ export GO_VERSION=1.15.3 GO_OS=linux GO_ARCH=amd64  
$ wget  
https://dl.google.com/go/go${GO_VERSION}.${GO_OS}-${GO_ARCH}.t  
ar.gz  
$ tar -C /usr/local/ -xvf go1.15.3.linux-amd64.tar.gz  
$ echo 'export GOPATH=${HOME}/go' >> ~/.bashrc  
$ echo 'export PATH=/usr/local/go/bin:${PATH}:${GOPATH}/bin'  
>> ~/.bashrc
```



```
$ source ~/.bashrc
```

Always as root user, install Singularity:

```
$ mkdir -p $GOPATH/src/github.com/sylabs
$ cd $GOPATH/src/github.com/sylabs
$ git clone https://github.com/sylabs/singularity.git
$ cd singularity/
$ go get -u -v github.com/golang/dep/cmd/dep
$ export SINGULARITY_VERSION=v3.6.1
$ git checkout ${SINGULARITY_VERSION}
$ ./mconfig
$ make -C builddir
$ make -C builddir install
```

Exit as root and log in as your local user. In the ~/.bashrc of your local user execute:

```
$ export PATH=/usr/local/bin:$PATH
$ export GOPATH=/root/go
$ export PATH=/usr/local/go/bin:${PATH}:${GOPATH}/bin
```

Further documentation about Singularity installation is available to <https://sylabs.io/guides/3.6/admin-guide/installation.html>

Windows or Mac Users

Please refer to

<https://sylabs.io/guides/3.6/admin-guide/installation.html#installation-on-windows-or-mac>

HUBS SET UP

In order to simplify the sharing of the container there are many hubs that allow you to upload your local recipes and images of containers for free.

Now we are going to set up the most important:

1. GitHub, <https://github.com/>

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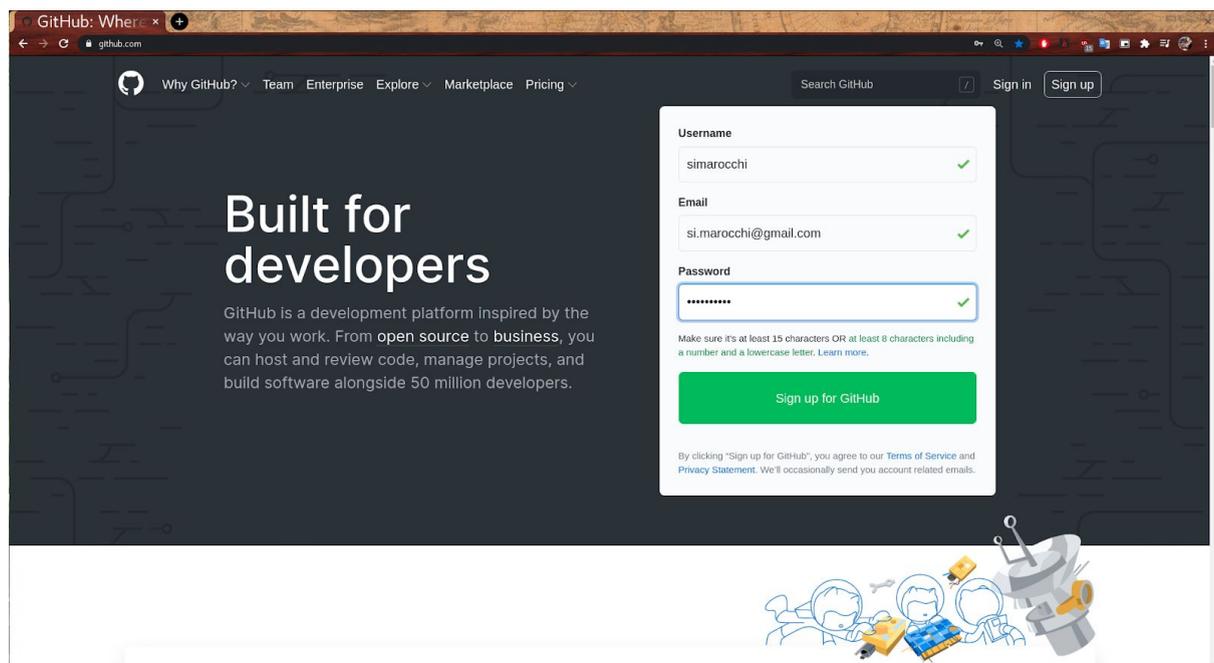
2. Docker Hub, <https://hub.docker.com/>
3. Singularity Hub, <https://singularity-hub.org/>

If you do not already have an account on these sites you can do the following procedure.

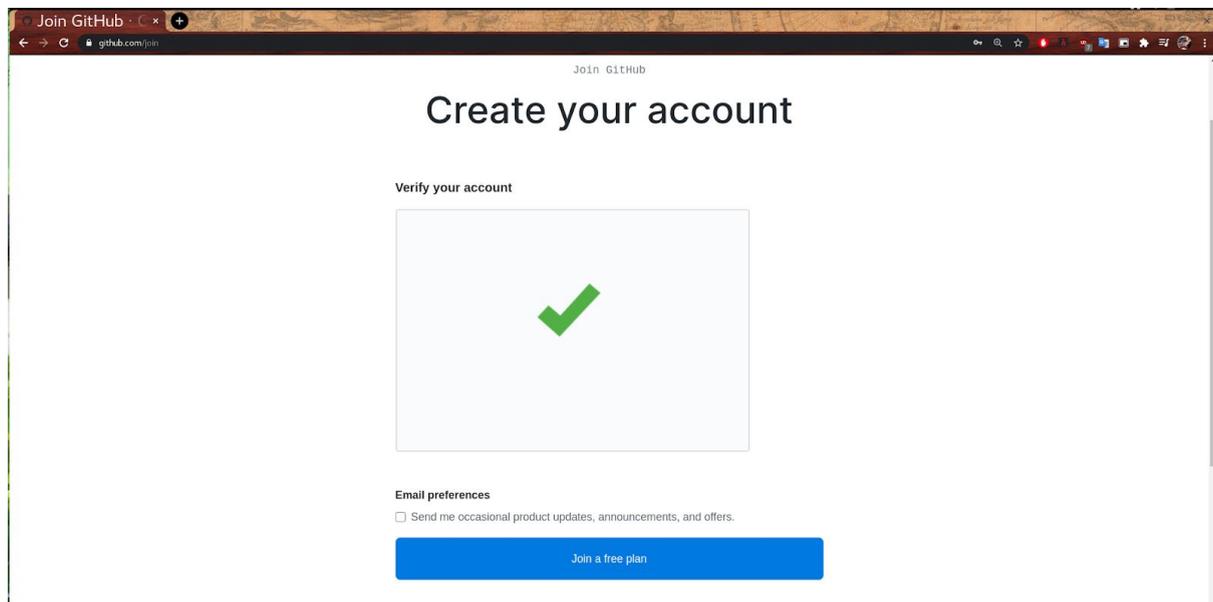
GIT HUB

Git is a distributed version-control system for tracking changes in source code during software development. The version-control system is quite powerful and a bit complex, in this tutorial we are going only to scratch all the potentials of this system. We are going to create your personal account in GitHub in order to have a place to save your container recipe files (as text files).

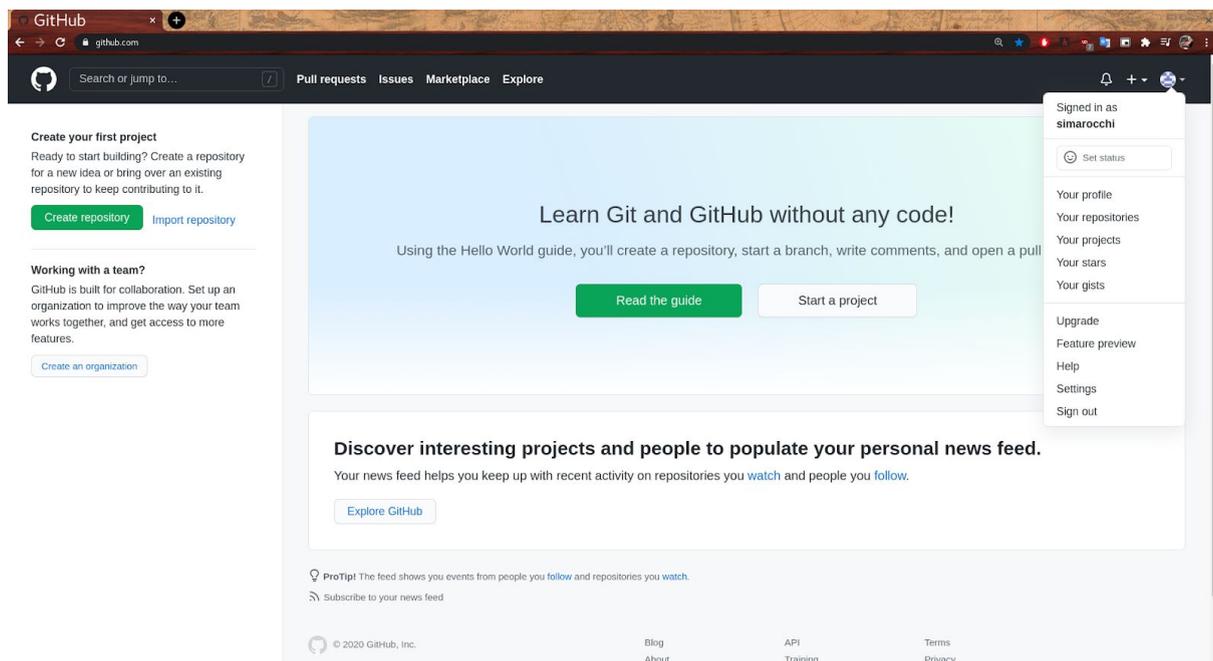
You have to sign up in the GitHub creating your own username and connecting it to your email



After the registration you will receive an email to your address to verify your new account. Do that and enjoy a free plan in GitHub.



At the end of the procedure if you login you should see the main window. From this page you can create your new repository where to put your code. So far your job is done with GitHub. Let's move to the next Hub.



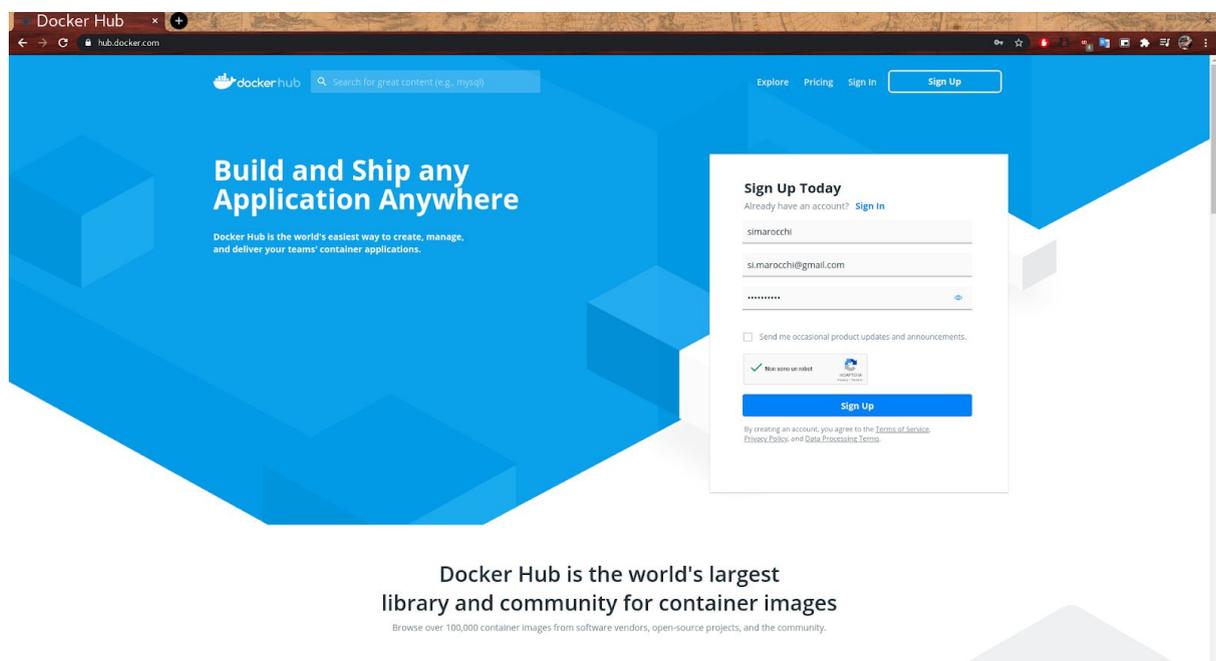
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DOCKER HUB

Docker Hub is a hosted repository service provided by Docker for finding and sharing container images with your team. Key features include: Private/Public Repositories: Push and pull container images. Automated Builds: Automatically build container images from GitHub (we will do this hands-on).

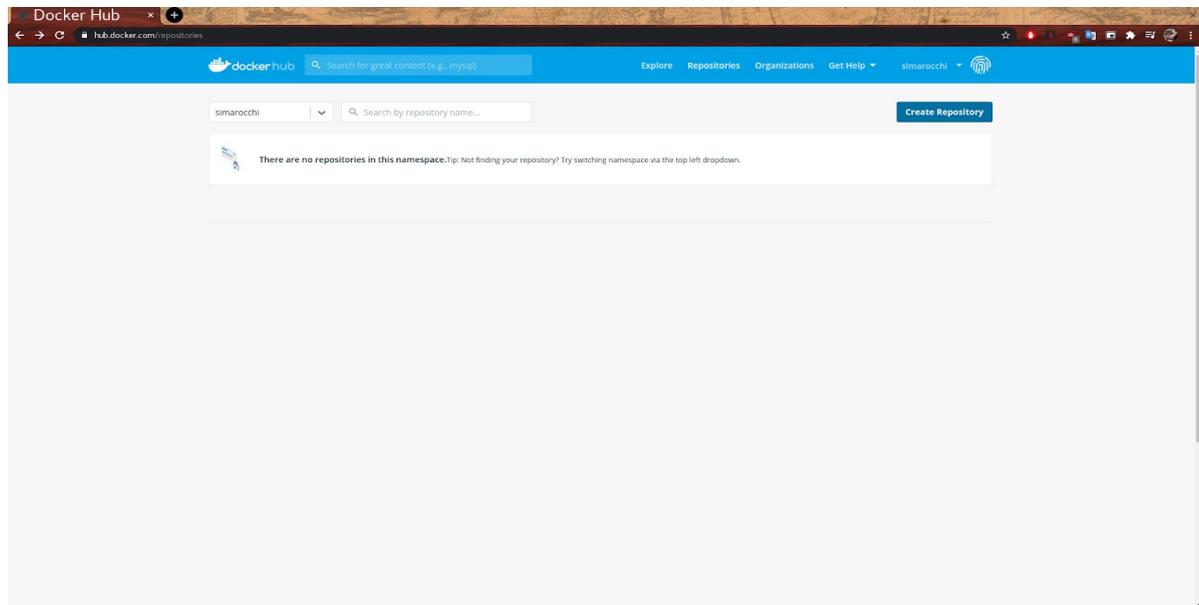
We are going to create your personal account in Docker Hub in order to have a place to save your container image files.

You have to sign up in the Docker Hub creating your own username and connecting it to your email.



After the registration you will receive an email to your address to verify your new account. Do that and enjoy a free plan in Docker Hub. At the end of the procedure if you login you should see the main window:

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From this page you can create your new repository where to put your images. So far your job is done with Docker Hub. Let's move to the next Hub.

SINGULARITY HUB

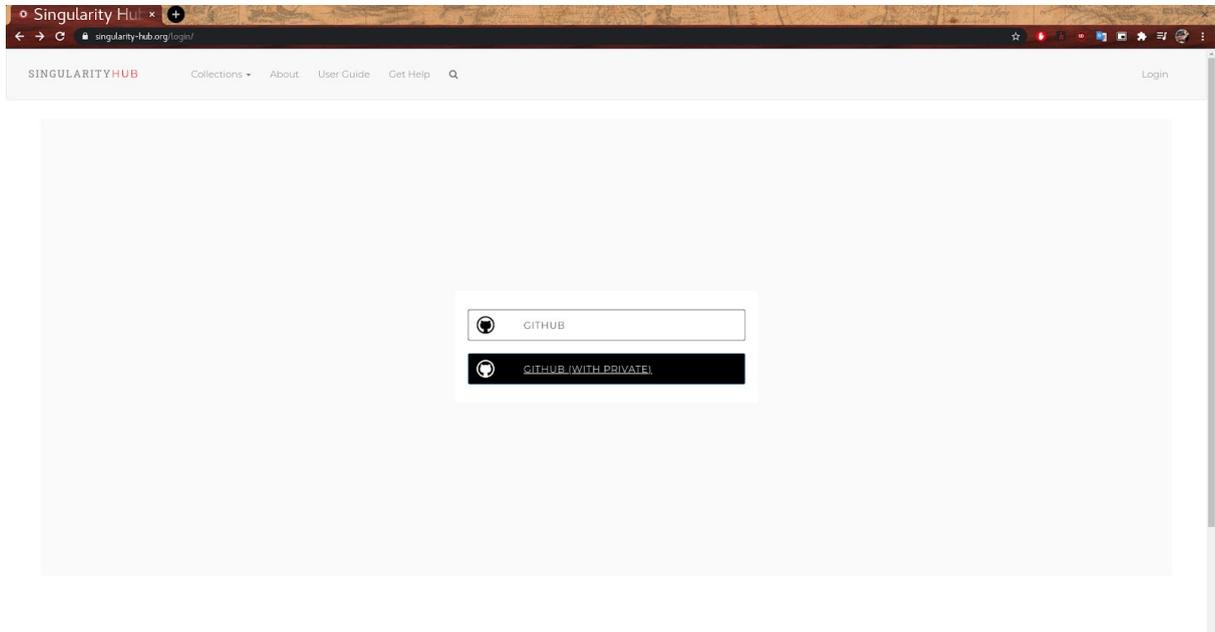
Singularity Hub is a hosted repository service provided by Singularity (pretty similar to Docker Hub) for finding and sharing container images with your team.

Key features include: private/public repositories; push and pull container images; image signature; automated builds: automatically build container images from GitHub (we will do this in the hands-on).

We are going to create your personal account in Singularity Hub in order to have a place to save your container image files.

You have to sign up in the Singularity Hub, connecting it to your email. You can also use your previous GitHub login to get the access also to Singularity Hub. Select the option "GITHUB (WITH PRIVATE)"

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At the end of the procedure if you login you should see the following window:

