



# USING GATE AND SINGULARITY ON CC

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*Cassandra Miller*

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# 1. GET DOCKER IMAGE

- First you need to pull the docker image using **singularity**
- CC does NOT have docker so the normal docker commands will not work!!
- This only works with a **public** docker repository

- First: SSH into Compute Canada (CC) and load singularity

```
cassandra$ ssh -Y camiller@cedar.compute canada.ca
```

```
[camiller@cedar1 ~]$ module load singularity/3.6
```

- We need to pull the docker file using singularity.
- Create a job to submit to CC clusters (I use Cedar cluster)
  - This won't work in the regular shell, because it takes up too much memory
- Example of bash file:

```
#!/bin/bash
#SBATCH --time=5:00:00
#SBATCH --mem=32G
singularity pull docker://ghcr.io/carluri/gate9.0:latest
```

- Anytime you want to submit a job to CC, you need to make a bash file like this.

Now submit job (which I titled PullDockerImage.sh)

```
[camiller@cedar1 scratch]$ sbatch PullDockerImage.sh
```



- The job might be killed if it runs out of time or if the memory is not high enough, if this happens just increase the time/memory and run again.
- If it works you will now have a .sif file, which you can run like any other executable file. When you run it, you will be inside the container:

```
[camiller@cedar1 scratch]$ ls *.sif
gate9.0_latest.sif
[camiller@cedar1 scratch]$ ./gate9.0_latest.sif
Singularity> ls ..
camiller  gateuser
Singularity> █
```

Notice that our location changed from [camiller@cedar1 scratch] to Singularity>

That's because we're inside the container, so we no longer can use CC commands (e.g. use "module load" or submit jobs)

**Issue:** when I am inside my Gate singularity container, I cannot access my CC scratch directory. I overcame this problem by creating a new directory "scratch2" and binding my scratch directory (in CC) to my scratch2 directory (in my singularity container) when I run my container. This is done using the "-B" command, which "binds" the locations:

```
[camiller@cedar1 ~]$ singularity run -B /home/camiller/scratch:/home/camiller/scratch2 gate9.0_latest.sif
```

(note that "singularity run file.sif" is identical to "./file.sif")

Now, files I create in the singularity container in the folder "scratch2" will appear in the "scratch" folder in my CC directory.

## 2. SUBMITTING JOBS

Inside the singularity container, you cannot submit batch jobs to the CC cluster. Instead, you need to use the “singularity exec” command to submit a job in the container from outside the container.



Simple example:

In my container, I want to enter the “gateuser” directory and display my current path. This doesn’t work outside of the container, because that path doesn’t exist:

```
[camiller@cedar1 ~]$ cd ../gateuser  
-bash: cd: ../gateuser: No such file or directory  
[camiller@cedar1 ~]$
```

Make a bash script with everything you want to do inside the singularity container (this script must be INSIDE container):

```
#!/bin/bash

#### bash file "myscript.sh"
cd ../gateuser
pwd
```

And you can run the following command on CC (NOT in singularity container)

```
[camiller@cedar1 ~]$ singularity exec --nv -B /home/camiller/scratch:/home/camiller/scratch2 gate9.0_latest.sif bash myscript.sh
/home/gateuser
[camiller@cedar1 ~]$
```

As you see, it worked because it outputted the directory (from pwd) even though we never went inside the container interactively.

Therefore, you can run whatever you want on singularity from your CC terminal, by writing a script detailing everything you want to do inside your container.

```
#!/bin/bash
#SBATCH --time=1:40:00
#SBATCH --mem=16G

singularity exec --nv -B /home/camiller/scratch:/home/camiller/scratch2 gate9.0_latest.sif bash whateverscript.sh
```

And run the above using “sbatch” as usual.

It also doesn't have to be “bash myfile.sh”, it can be any command, for example “python myfile.py”, or whatever.