



# DNA Club

Using CAW with Singularity containers on UPPMAX clusters

---

Maxime Garcia

2017-20-09



# What is Singularity?



<http://singularity.lbl.gov/>

<https://singularity-hub.org/>

- Docker-like containers technology
- Specific for HPC environment

# What is Singularity?



<http://singularity.lbl.gov/>

<https://singularity-hub.org/>

- Docker-like containers technology
- Specific for HPC environment
- Without the root user security problem

# What is Singularity?



<http://singularity.lbl.gov/>

<https://singularity-hub.org/>

- Docker-like containers technology
- Specific for HPC environment
- Without the root user security problem
- Singularity hub offers a Docker hub like repository
- Singularity containers can be pulled from Docker hub

# What is Singularity?



<http://singularity.lbl.gov/>

<https://singularity-hub.org/>

- Docker-like containers technology
- Specific for HPC environment
- Without the root user security problem
- Singularity hub offers a Docker hub like repository
- Singularity containers can be pulled from Docker hub
- Supported by Nextflow

## **Why would we want to use that?**

---

- For a better control

## Why would we want to use that?

---

- For a better control
  - of every tool used
  - of every version used

## Why would we want to use that?

---

- For a better control
  - of every tool used
  - of every version used
- For a better reproducibility

## Why would we want to use that?

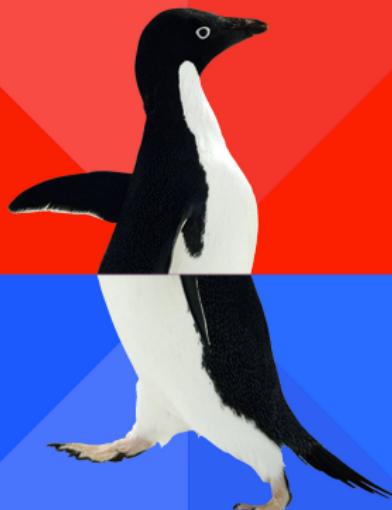
---

- For a better control
  - of every tool used
  - of every version used
- For a better reproducibility

Containerization is not only portable but also reproducible.

We can do everything!

WE CAN USE ANY VERSION  
OF ANY TOOL WE WANT



WE ARE RESPONSIBLE FOR  
EVERY TOOL WE WANT

# The CAW-containers repository

README.md



## Containers for CAW

[release v1.1](#) [license MIT License](#) [nextflow >0.23.2](#) [chat on gitter](#) [build passing](#)

CAW is a complete open source pipeline to detect somatic variants from WGS data developed at the [National Genomics Infrastructure](#) at [SciLifeLab Stockholm](#), Sweden.

For further information/help contact: [maxime.garcia@scilifelab.se](mailto:maxime.garcia@scilifelab.se) or [szilveszter.juhos@scilifelab.se](mailto:szilveszter.juhos@scilifelab.se), or join the gitter chat: [gitter.im/SciLifeLab/CAW](https://gitter.im/SciLifeLab/CAW)

### Documentation

This repo comes with documentation about the different containers, found in the `doc/` directory:

1. Documentation about containers
2. Documentation about building

### Author

• Maxime Garcia

---

**SciLifeLab**



NATIONAL GENOTYPE & GENOMICS INFRASTRUCTURE



NATIONAL BIOINFORMATICS INFRASTRUCTURE SWEDEN

## How many containers?

---

## How many containers?

---

- One container for everything

## How many containers?

---

- One container for everything
- Several containers (one for each process)

# The One Script

---

## SciLifeLab/CAW-containers

- 24 different Docker containers for all the different processes

# The One Script

---

## SciLifeLab/CAW-containers

- 24 different Docker containers for all the different processes
- One Script to build them all,

# The One Script

---

SciLifeLab/CAW-containers

- 24 different Docker containers for all the different processes
- One Script to build them all,

One Script to push them

# The One Script

---

## SciLifeLab/CAW-containers

- 24 different Docker containers for all the different processes
- One Script to build them all,

One Script to push them

- One Script to pull them all,

# The One Script

---

## SciLifeLab/CAW-containers

- 24 different Docker containers for all the different processes
- One Script to build them all,

One Script to push them

- One Script to pull them all,

and with Singularity run them

## Inside the script

---

SciLifeLab/CAW-containers/main.nf

```
docker build -t $repository/$container:$tag \
$baseDir/containers/$container/.
```

```
docker push $repository/$container:$tag
```

```
singularity pull --name $container-${tag}.img \
docker://$repository/$container:$tag
```

## Nextflow and Singularity for the win

---



- Nextflow natively support Singularity



- Nextflow natively support Singularity
- Easy configuration



- Nextflow natively support Singularity
- Easy configuration
- Automatic pull of the containers

## Easy configuration

SciLifeLab/CAW/configuration/singularity.config

```
singularity {
    enabled = true
}
process {
    $RunFastQC.container      = 'docker://maxulysse/fastqc:1.1'
    $RunFreeBayes.container   = 'docker://maxulysse/freebayes:1.1'
    $RunGenotypeGVCFs.container = 'docker://maxulysse/gatk:1.1'
    $RunManta.container       = 'docker://maxulysse/runmanta:1.1'
    $RunMultiQC.container     = 'docker://maxulysse/multiqc:1.1'
    $RunMutect1.container     = 'docker://maxulysse/mutect1:1.1'
}
```

## Easy configuration

SciLifeLab/CAW/configuration/singularity.config

```
singularity {
    enabled = true
}
process {
    $RunFastQC.container      = 'docker://maxulysse/fastqc:1.1'
    $RunFreeBayes.container   = 'docker://maxulysse/freebayes:1.1'
    $RunGenotypeGVCFs.container = 'docker://maxulysse/gatk:1.1'
    $RunManta.container       = 'docker://maxulysse/runmanta:1.1'
    $RunMultiQC.container     = 'docker://maxulysse/multiqc:1.1'
    $RunMutect1.container     = 'docker://maxulysse/mutect1:1.1'
}

process.container = 'shub://MaxUlysse/shubcontainer'

export NXF_SINGULARITY_CACHEDIR=$HOME/.singularity
```

## What to do on a secure cluster?

---

- How about running CAW with Singularity on Bianca or Irma?

## What to do on a secure cluster?

---

- How about running CAW with Singularity on Bianca or Irma?
- No automatic pull of the containers

## What to do on a secure cluster?

---

- How about running CAW with Singularity on Bianca or Irma?
- No automatic pull of the containers
- The configuration is still easy

## Still an easy configuration

```
SciLifeLab/CAW/configuration/singularity-download.config

singularity {
    enabled = true
}
process {
    $RunFastQC.container      = 'containers/fastqc-1.1.img'
    $RunFreeBayes.container   = 'containers/freebayes-1.1.img'
    $RunGenotypeGVCFs.container = 'containers/gatk-1.1.img'
    $RunManta.container       = 'containers/runmanta-1.1.img'
    $RunMultiQC.container     = 'containers/multiqc-1.1.img'
    $RunMutect1.container     = 'containers/mutect1-1.1.img'
}

export NXF_SINGULARITY_CACHEDIR=$HOME/.singularity

process.container = '$NXF_SINGULARITY_CACHEDIR/container.img'
```

## How to get the containers?

---

- Use the script that does the thing

## How to get the containers?

---

- Use the script that does the thing
- To pull all containers from Docker-hub into Singularity containers

## How to get the containers?

---

- Use the script that does the thing
- To pull all containers from Docker-hub into Singularity containers
- Transfer the containers to the secure cluster

## One last detail

---

- Do not forget to create the UPPMAX specific directories in the containers

## One last detail

---

- Do not forget to create the UPPMAX specific directories in the containers
- /pica
- /proj
- /sw

# Let the magic happen

---

SciLifeLab/CAW/main.nf

```
nextflow run ~/CAW/main.nf --project project --step preprocessing \
--genome GRCh38 --sample sample.tsv -profile singularityLocal
```

# Using parallelization to do multiple tests

## SciLifeLab/CAW/.travis.yml

```
sudo: required
language: java
jdk: openjdk8
services:
- docker
env:
- NXF_VER=0.25.6 PROFILE=dockerTest TEST=ANNOTATEVEP TOOL_INSTALL=nextflow
- NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularityTest TEST=ANNOTATESNPEFF TOOL_INSTALL=all
- NXF_VER=0.25.6 PROFILE=dockerTest TEST=ANNOTATESNPEFF TOOL_INSTALL=nextflow
- NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularityTest TEST=RECALIBRATE TOOL_INSTALL=all
- NXF_VER=0.25.6 PROFILE=dockerTest TEST=RECALIBRATE TOOL_INSTALL=nextflow
- NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularityTest TEST=REALIGN TOOL_INSTALL=all
- NXF_VER=0.25.6 PROFILE=dockerTest TEST=REALIGN TOOL_INSTALL=nextflow
- NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularityTest TEST=MAPPING TOOL_INSTALL=all
- NXF_VER=0.25.6 PROFILE=dockerTest TEST=MAPPING TOOL_INSTALL=nextflow

install: # Install Nextflow (and Singularity if needed)
- "./scripts/install.sh --tool $TOOL_INSTALL"

script:
- "./scripts/test.sh --profile $PROFILE --test $TEST"
```

# All your test are belong to us.

## SciLifeLab / CAW

build passing

Current Branches Build History Pull Requests Build #433 More options

✓ Pull Request #457 Update Manta and Strelka

Commit 2be368b ↗  
#457: Update Manta and Strelka ↗  
Branch master ↗  
Maxime Garcia authored and committed

#433 passed  
Ran for 22 min 12 sec  
Total time 2 hrs 13 min 2 sec  
about 3 hours ago

Restart build

### Build Jobs

✓ # 433.1	⚙️ ↗ JDK: openjdk8	NXF_VER=0.25.6 PROFILE=dockerTest TEST=ANNOT	22 min 12 sec	↻
✓ # 433.2	⚙️ ↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularit	23 min 57 sec	↻
✓ # 433.3	⚙️ ↗ JDK: openjdk8	NXF_VER=0.25.6 PROFILE=dockerTest TEST=ANNOT	22 min 6 sec	↻
✓ # 433.4	⚙️ ↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularit	11 min 53 sec	↻
✓ # 433.5	⚙️ ↗ JDK: openjdk8	NXF_VER=0.25.6 PROFILE=dockerTest TEST=RECALI	11 min 15 sec	↻
✓ # 433.6	⚙️ ↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularit	11 min 29 sec	↻
✓ # 433.7	⚙️ ↗ JDK: openjdk8	NXF_VER=0.25.6 PROFILE=dockerTest TEST=REALIG	9 min 43 sec	↻
✓ # 433.8	⚙️ ↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularit	14 min 13 sec	↻
✓ # 433.9	⚙️ ↗ JDK: openjdk8	NXF_VER=0.25.6 PROFILE=dockerTest TEST=MAPPIN	6 min 14 sec	↻

## The List of People Involved

---

Sebastian DiLorenzo	Monica Nistèr
Jesper Eisfeldt	Björn Nystedt
Maxime Garcia	Pall Olason
Szilveszter Juhos	Markus Ringnér
Max Käller	Pelin Sahlén
Malin Larsson	Johanna Sandgren
Marcel Martin	Teresita Díaz De Ståhl
Markus Mayrhofer	

## Where to find us?

- We are on the SciLifeLab Slack  
#cancer-pipeline

## Where to find us?

- We are on the SciLifeLab Slack  
#cancer-pipeline
- We have a gitter channel  
<https://gitter.im/SciLifeLab/CAW>

# Where to find us?

- We are on the SciLifeLab Slack  
`#cancer-pipeline`
- We have a gitter channel  
<https://gitter.im/SciLifeLab/CAW>
- Our code is hosted on Github  
<https://github.com/SciLifeLab/CAW>

# Any questions?



# Any questions?

