



Cancer Analysis Workflow

Yes we can run it on Irma with Singularity containers

Maxime Garcia

2017-08-29



What is Singularity?



- Docker-like containers technology
- Specific for HPC environment

What is Singularity?



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

What is Singularity?



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

What is Singularity?



- Docker-like containers technology
- Specific for HPC environment
- Without the root user security problem
- Supported by Nextflow
- Can pull containers from Docker-hub

Why would we want to do that?

- For a better control

Why would we want to do that?

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

Why would we want to do that?

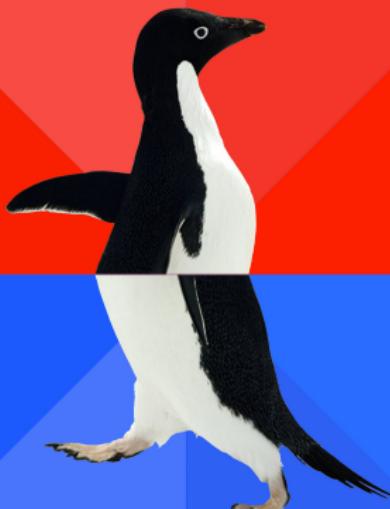
- For a better control
- of every tool used
- of every version used
- For a better reproducibility

Why would we want to do that?

- For a better control
- of every tool used
- of every version used
- For a better reproducibility
- Containerization is reproducible and portable

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 or szilveszter.juhos@scilifelab.se, or join the gitter chat: 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

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 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 {
    autoMounts = true
    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 {
    autoMounts = true
    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'
```

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 {
    autoMounts = true
    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'
}
```

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

One last detail

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

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 SGT_VER=2.3.1 TEST=ANNOTATE PROFILE=singularity
- NXF_VER=0.25.6 SGT_VER=2.3.1 TEST=ANNOTATE PROFILE=docker
- NXF_VER=0.25.6 SGT_VER=2.3.1 TEST=RECALIBRATE PROFILE=singularity
- NXF_VER=0.25.6 SGT_VER=2.3.1 TEST=RECALIBRATE PROFILE=docker
- NXF_VER=0.25.6 SGT_VER=2.3.1 TEST=REALIGN PROFILE=singularity
- NXF_VER=0.25.6 SGT_VER=2.3.1 TEST=REALIGN PROFILE=docker
- NXF_VER=0.25.6 SGT_VER=2.3.1 TEST=MAPPING PROFILE=singularity
- NXF_VER=0.25.6 SGT_VER=2.3.1 TEST=MAPPING PROFILE=docker

install: # Install Nextflow
- ./scripts/install.sh --tool nextflow

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

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  #433 passed 

↳ Commit 2be368b 
↳ #457: Update Manta and Strelka 
↳ Branch master 

 Maxime Garcia authored and committed 

Build Jobs

✓ # 433.1	 ↳ JDK: openjdk8	 NXF_VER=0.25.6 PROFILE=dockerTest TEST=ANNOTATION  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=ANNOTATION  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=RECALIBRATION  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=REALIGNMENT  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=MAPPING  6 min 14 sec 

The List of People Involved

Sebastian DiLorenzo

Jesper Eisfeldt

Maxime Garcia

Szilveszter Juhos

Max Käller

Malin Larsson

Marcel Martin

Monica Nistèr

Björn Nystedt

Pall Olason

Pelin Sahlén

Johanna Sandgren

Teresita Díaz De Ståhl

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?

