



Cancer Analysis Workflow

Yes we can run it on Irma/Bianca with Singularity containers

Maxime Garcia

2017-20-09



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- Specific for HPC environment

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

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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!



The CAW-containers repository

README.md



Containers for CAW

[release v1.0](#) [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

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SciLifeLab/CAW-containers

- 24 different Docker containers for all the different processes

The One Script

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- One Script to build them all,

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- 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
```



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- 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

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    $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?

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

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- 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

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- /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=singularityTest TOOL_INSTALL=all
  - NXF_VER=0.25.6 TEST=ANNOTATE PROFILE=dockerTest TOOL_INSTALL=nextflow
  - NXF_VER=0.25.6 SGT_VER=2.3.1 TEST=RECALIBRATE PROFILE=singularityTest TOOL_INSTALL=all
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  - NXF_VER=0.25.6 TEST=MAPPING PROFILE=dockerTest 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 #344

More options



✓ Pull Request #426 Install Singularity on TravisCI only when necessary

344 passed

Restart build

-o Commit bfd33b1 ↗

🕒 Ran for 23 min 27 sec

↳ #426: Install Singularity on TravisCI only when necessary ↗

⌚ Total time 1 hr 29 min 43 sec

↳ Branch master ↗

🕒 about 6 hours ago

Maxime Garcia authored and committed

Build Jobs

✓ # 344.1	↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularit	⌚ 16 min 53 sec	
✓ # 344.2	↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=travis TES	⌚ 15 min 20 sec	
✓ # 344.3	↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularit	⌚ 11 min 23 sec	
✓ # 344.4	↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=travis TES	⌚ 11 min	
✓ # 344.5	↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularit	⌚ 11 min 37 sec	
✓ # 344.6	↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=travis TES	⌚ 10 min 59 sec	
✓ # 344.7	↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=singularit	⌚ 6 min 38 sec	
✓ # 344.8	↗ JDK: openjdk8	NXF_VER=0.25.6 SGT_VER=2.3.1 PROFILE=travis TES	⌚ 5 min 53 sec	

The List of People Involved

Sebastian DiLorenzo	Monica Nistér
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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

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- We have a gitter channel
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- Our code is hosted on Github
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Any questions?



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