



DNA Club

Using CAW with Singularity containers on UPPMAX clusters

Maxime Garcia

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

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

- Docker-like containers technology
- Specific for HPC environment

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- Supported by Nextflow

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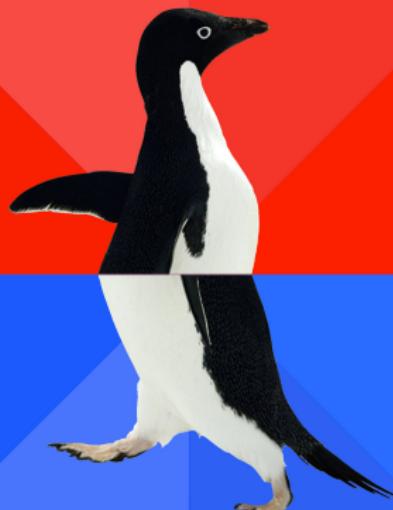
Why would we want to use that?

- 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 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

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

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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
```

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

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    $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 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
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- 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  #433 passed 

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

⌚ about 3 hours ago 

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	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

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#cancer-pipeline
- 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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