Introduction to automation using Nextflow: *A tutorial through examples*

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Outline

Introduction to Nextflow

Introduction to Nextflow

Introduction

Resources

- `https://github.com/phelelani/nf-tutorial`

Workflow Languages

Many scientific applications require

- Multiple data files
- Multiple applications
- Perhaps different parameters

General purpose languages not well suited

- Too low a level of abstraction
- Does not separate workflow from application
- Not reproducible

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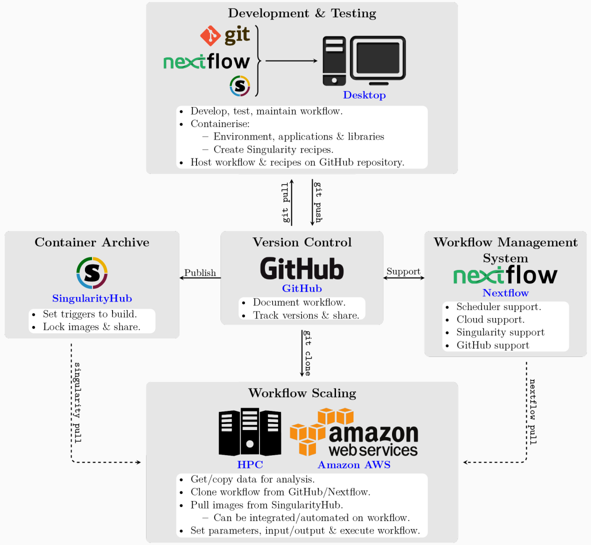
Development & Testing
git
nextflow
Desktop
• Develop, test, maintain workflow.
• Containerise:
– Environment, applications & libraries
– Create Singularity recipes.
• Host workflow & recipes on GitHub repository.
git pull
git push
Container Archive
SingularityHub
• Set triggers to build.
• Lock images & share.
Publish
Version Control
GitHub
GitHub
• Document workflow.
• Track versions & share.
Support
Workflow Management System
nextflow
Nextflow
• Scheduler support.
• Cloud support.
• Singularity support
• GitHub support
git clone
singularity pull
nextflow pull
Workflow Scaling
HPC
amazon web services
Amazon AWS
• Get/copy data for analysis.
• Clone workflow from GitHub/Nextflow.
• Pull images from SingularityHub.
– Can be integrated/automated on workflow.
• Set parameters, input/output & execute workflow.

Nextflow

Groovy-based language

- Expressing workflows
- Portable
    - works on most Unix-like systems
- Very easy to install
    - NB: requires Java 7, 8
- Scalable
- Supports Docker/Singularity
- Supports a range of scheduling systems

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Key concepts of Nextflow

- **Processes**:
  - actual work being done (usually simple).
  - call program that does the analysis.
- **Channels**:
  - for communication between processes.
  - handles inputs and outputs.
- When all inputs ready, process is executed.
- Each process runs in its own directory (files are staged).
- Supports resumption of previous partial runs.

Introduction to Nextflow

Nextflow Script

Exercise 1

You have an input file with 6 columns (see below), where column 2 is an ”index” column. Identify rows that have identical indexes (column 2) and remove them from the file.

Your input file looks like this:

```
11   11:189256   0   189256   A   G
11   11:193788   0   193788   T   C
11   11:194062   0   194062   T   C
11   11:194228   0   194228   A   G
11   11:193788   0   193788   A   C
```

Simple Example: Using BASH

Input is a file

- With 6 columns
- Column 2 is an index column
- Identify rows with identical field 2
- Remove identical rows

```
11   11:189256   0   189256   A   G
11   11:193788   0   193788   T   C
11   11:194062   0   194062   T   C
11   11:194228   0   194228   A   G
11   11:193788   0   193788   A   C
```

Using BASH:

```
cut -f 2 data/11.bim  | sort | uniq -d  > dups
grep -v -f dups data/11.bim > 11.clean
```

Simple Example: Using `nextflow`

```
#!/usr/bin/env nextflow
nextflow.enable.dsl=2

input_ch = Channel.fromPath("data/11.bim")

process getIDs {
    input:
    path(input_ch)

    output:
    path("ids"), emit: id_ch
    path("11.bim"), emit: orig_ch

    """
    cut -f 2 ${input_ch} | sort > ids
    """
}

process getDups {
    input:
    path(id_ch)

    output:
    path("dups"), emit: dups_ch

    """
    uniq -d ${id_ch} > dups
    touch ignore
    """
}
```

Simple Example: Using nextflow

```
#!/usr/bin/env nextflow
nextflow.enable.dsl=2

input_ch = Channel.fromPath("data/11.bim")

process getIDs {
    input:
    path(input_ch)

    output:
    path("ids"), emit: id_ch
    path("11.bim"), emit: orig_ch

    """
    cut -f 2 ${input_ch} | sort > ids
    """
}

process getDups {
    input:
    path(id_ch)

    output:
    path("dups"), emit: dups_ch

    """
    uniq -d ${id_ch} > dups
    touch ignore
    """
}
```

```
process removeDups {
    input:
    path(dups_ch)
    path(orig_ch)

    output:
    path("clean.bim"), emit: output

    """
    grep -v -f ${dups_ch} ${orig_ch} > clean.bim
    """
}

workflow {
    getIDs(input_ch)
    getDups(getIDs.out.id_ch)
    removeDups(getDups.out.dups_ch, getIDs.out.orig_ch).
       subscribe { print "Done!" }
}
```

Simple Example: Using `nextflow`

```
$ nextflow run cleandups.nf

N E X T F L O W  ~  version 19.04.1
Launching `cleandups.nf` [soggy_jennings] - revision: 795e2aa39d
[warm up] executor > local
executor >  local (3)
[84/7e1ad1] process > getIDs     [100%] 1 of 1 ✓
[19/cc8bf9] process > getDups    [100%] 1 of 1 ✓
[f9/ed086d] process > removeDups [100%] 1 of 1 ✓
Completed at: 31-Jul-2019 09:00:50
Duration    : 1.5s
CPU hours   : (a few seconds)
Succeeded   : 3
```

```
|--work
|  |--90
|  |  |--cebf3649d883f88381e32b4912b560
|  |  |  |--ids -> /Users/phele/day4/work/b3/aa0380f2a1bca447259b7ffd390083/ids
|  |  |  |--ignore
|  |--9c
|  |  |--e0cb7d8d26682d7d4a1c44392f2bb3
|  |  |  |--11.bim -> /Users/phele/day4/data/11.bim
|  |  |  |--clean.bim
|  |  |  |--dups -> /Users/phele/day4/work/90/cebf3649d883f88381e32b4912b560/dups
|  |--b3
|  |  |--aa0380f2a1bca447259b7ffd390083
|  |  |  |--11.bim -> /Users/phele/day4/data/11.bim
|  |  |  |--ids
```

Exercise 2

Change the script so that you use `stdin` or `stdout` in the `getIDs` and `getDups` processes to avoid the use of the temporary file ids. You can see the solution: ex2-cleandups-stdin.nf!.

Introduction to Nextflow

Partial Execution

Partial Execution

If execution of workflow is only partial

- Because of error
- Only need to resume from process that failed

```
nextflow run cleandups.nf -resume
```

Introduction to Nextflow

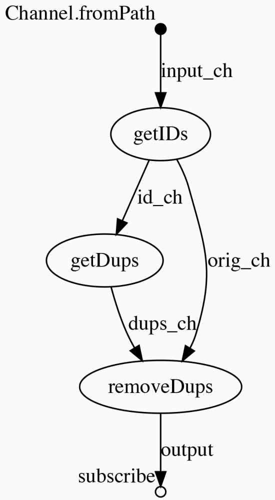
Visualising the Workflow

Visualising the Workflow

Nextflow supports several visualisation tools:

-with-dag

```
nextflow run cleandups.nf -with-dag <file-name>
```



Visualising the Workflow

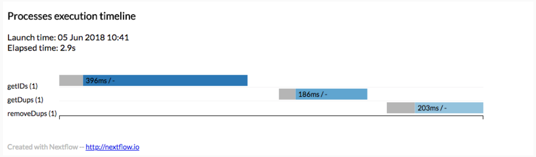
Nextflow supports several visualisation tools:

-with-dag

```
nextflow run cleandups.nf -with-dag <file-name>
```

-with-timeline

```
nextflow run cleandups.nf -with-timeline <file-name>
```


Processes execution timeline

Launch time: 05 Jun 2018 10:41
Elapsed time: 2.9s

Created with Nextflow -- http://nextflow.io

Visualising the Workflow

Nextflow supports several visualisation tools:

-with-dag

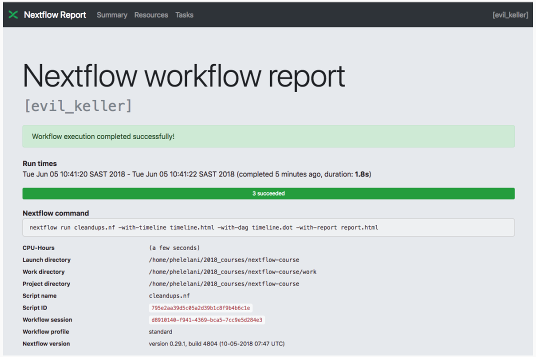
```
nextflow run cleandups.nf -with-dag <file-name>
```

-with-timeline

```
nextflow run cleandups.nf -with-timeline <file-name>
```

-with-report

```
nextflow run cleandups.nf -with-report <filename>
```



Nextflow workflow report

[evil_keller]

Workflow execution completed successfully!

Run times

Tue Jun 05 10:41:20 SAST 2018 - Tue Jun 05 10:41:22 SAST 2018 (completed 5 minutes ago, duration: **1.8s**)

3 succeeded

Nextflow command

```
nextflow run cleandups.nf -with-timeline timeline.html -with-dag timeline.dot -with-report report.html
```

CPU-Hours	(a few seconds)
Launch directory	/home/phelelani/2018_courses/nextflow-course
Work directory	/home/phelelani/2018_courses/nextflow-course/work
Project directory	/home/phelelani/2018_courses/nextflow-course
Script name	cleandups.nf
Script ID	795e2aa39d5c05a2d39b1c8f9b4b6c1e
Workflow session	d8910140-f941-4369-bca5-7cc9e5d284e3
Workflow profile	standard
Nextflow version	version 0.29.1, build 4804 (10-05-2018 07:47 UTC)

Groovy

Groovy

Nextflow is a DSL built with Groovy

- Can inter-mix Nextflow, Groovy and Java code.
- Very powerful, flexible.
- Don’t need to know much (any?) Groovy but a little knowledge is a powerful thing

Groovy

Groovy Closures

Groovy: Closures

Closures are anonymous functions

- Similar to lambdas in Python
- Don’t want the overhead of naming a function we only use once
- Typically use with higher-order functions
    - Functions that take other functions as arguments
- Very powerful and useful

Syntax for a closure that takes one argument:

```
{ parm -> expression }
```

Groovy: Closures

Closures are anonymous functions

- Similar to lambdas in Python
- Don't want the overhead of naming a function we only use once
- Typically use with higher-order functions
  - Functions that take other functions as arguments
- Very powerful and useful

Syntax for a closure that takes one argument:

```
{ parm -> expression }
```

```
{ a -> a*a } (3)

{ a -> a*a+7*a - 2 } (3)

for (n in 1..5) print( {it*it} (n));

{ x, y ->  Math.sqrt(x*x + y*y) } (3,4)

int doX(f, nums) {
  sum=0;
  for ( n in nums ) {
    sum = sum+f(n);
  }
  return sum
}

print doX ( {a->a},   [4,5,16] );

print doX ( {a->a*a}, [4,5,16] );

print doX ( { it*it }, [4,5,16]);

m=10

print doX({a->m*a+2}, [1,2,3])
```

Exercise 3

Look at the sample Groovy code: ex3-groovy.nf. Try to understand and execute on your machine (using the Groovy Console)

Generalising and Extending

Extending the Example

- Parameterise the input
- Want output to go to convenient place
- Workflow takes in multiple input files – processes are executed on each in turn.
- Complication : may need to carry the base name of the input to the final output;
- Can repeat some steps for different parameters.

Generalising and Extending

Parameters

Parameters

In Nextflow file:

```
input_ch = Channel.fromPath(params.data)
```

And run it like this

```
nextflow run phylo1.nf --data data/polyseqs.fa
```

Generalising and Extending

Channels

Data Types in Channels

Channels support different types:

- path
- stdin
- env
- tuple

Many, many operations you can do on channels and their contents

bind	buffer	close
filter	map/reduce	group
join, merge	mix	copy
split	spread	fork
count	min/max/sum	print/view

Creating Channels

```
Channel.create()
Channel.empty
Channel.from("blast","plink")
Channel.fromPath("data/*.fa")
Channel.fromFilePairs("data/{YRI,CEU,BEB}.*")
Channel.watchPath("*fa")
```

Generalising and Extending

Generalising Our Example

Workflow: Multiple Inputs

```
#!/usr/bin/env nextflow
nextflow.enable.dsl=2

params.data_dir = "data"
input_ch = Channel.fromPath("${params.data_dir}/*.bim")

process getIDs {
    input:
    path(input)

    output:
    path("${input.baseName}.ids"), emit: id_ch
    path("${input}"), emit: orig_ch

    """
    cut -f 2 ${input} | sort > ${input.baseName}.ids
    """
}

process getDups {
    input:
    path(input)

    output:
    path("${input.baseName}.dups"), emit: dups_ch

    """
    uniq -d ${input} > "${input.baseName}.dups"
    touch ignore
    """
}
```

Workflow: Multiple Inputs

```
#!/usr/bin/env nextflow
nextflow.enable.dsl=2

params.data_dir = "data"
input_ch = Channel.fromPath("${params.data_dir}/*.bim")

process getIDs {
    input:
    path(input)

    output:
    path("${input.baseName}.ids"), emit: id_ch
    path("${input}"), emit: orig_ch

    """
    cut -f 2 ${input} | sort > ${input.baseName}.ids
    """
}

process getDups {
    input:
    path(input)

    output:
    path("${input.baseName}.dups"), emit: dups_ch

    """
    uniq -d ${input} > "${input.baseName}.dups"
    touch ignore
    """
}
process removeDups {
    publishDir "output", pattern: "${badids.baseName}.bim",
       overwrite:true, mode:'copy'

    input:
    path(badids)
    path(orig)

    output:
    path("${badids.baseName}_clean.bim"), emit: cleaned_ch

    """
    grep -v -f ${badids} ${orig} > ${badids.baseName}_clean.bim
    """
}

workflow {
    getIDs(input_ch)
    getDups(getIDs.out.id_ch)
    removeDups(getDups.out.dups_ch, getIDs.out.orig_ch)
}
```

Workflow: Multiple Inputs

```
$ nextflow run cleandups.nf

Launching `cleandups.nf` [distracted_hodgkin] - revision: 29fdb384a6
[warm up] executor > local
executor >  local (9)
[1a/431eb7] process > getIDs     [100%] 3 of 3 ▯
[cc/fc0aaa] process > getDups    [100%] 3 of 3 ▯
[03/c31154] process > removeDups [100%] 3 of 3 ▯
Completed at: 31-Jul-2019 10:26:23
Duration    : 2s
CPU hours   : (a few seconds)
Succeeded   : 9
```

Exercise 4

Now try adding a process to our Nextflow example and for splitting the file but using different split values (solution: ex4-cleandups-multi-params.nf).

Workflow: Multiple Parameters

Now try splitting the file but use different split values

```
split  -l 400 data.txt dataX
```

will produce files dataXaa, dataXab, dataXac and so on ...

Try:

```
splits = [400,500,600]

process splitIDs  {
  input:
  path(bim)
  each split

  output:
  path("*-$split-*"), emit: output_ch

  """
  split -l ${split} ${bim} ${bim.baseName}-$split-
  """
}
```

Have a look at the modified Nextflow script: ex4-cleandups-multi-params-mod.nf.

Generalising and Extending

Managing Grouped Files

Grouped Files

Use PLINK as an example.

```
## Short version of the command
plink --bfile /path/YRI --freq --out /tmp/YRI

## Long version of the command
plink --bed YRI.bed \
    --bim YRI.bim \
    --fam YRI.fam \
    --freq \
    --out /tmp/YRI
```

Problem:

- Pass the files on another channel(s) to be staged
- Pass the base name as value/or work it out

Pros/Cons

- Simple
- Need extra channel/some gymnastics

Grouped Files

Use `PLINK` as an example.

```
## Short version of the command
plink --bfile /path/YRI --freq --out /tmp/YRI

## Long version of the command
plink --bed YRI.bed \
    --bim YRI.bim \
    --fam YRI.fam \
    --freq \
    --out /tmp/YRI
```

Problem:

- Pass the files on another channel(s) to be staged
- Pass the base name as value/or work it out

Pros/Cons

- Simple
- Need extra channel/some gymnastics

RECAP CLOSURES

Simply, a *closure* is an anonymous function

- Code wrapped in braces {, }
- Default argument called *it*

```
[1,2,3].each { print it * it }
[1,2,3].each { num -> print num * num }
```

Grouped Files - Version 1: map

```
#!/usr/bin/env nextflow
nextflow.enable.dsl=2

params.dir = "data/pops/"
dir = params.dir
params.pops = ["YRI","CEU","BEB"]

Channel
    .from(params.pops)
    .map { pop ->
        [ file("$dir/${pop}.bed"),
          file("$dir/${pop}.bim"),
          file("$dir/${pop}.fam")]
    }
    .set { plink_data }

plink_data.subscribe { println "$it" }
```

Grouped Files - Version 1: map

```
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nextflow.enable.dsl=2

params.dir = "data/pops/"
dir = params.dir
params.pops = ["YRI","CEU","BEB"]

Channel
    .from(params.pops)
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        [ file("$dir/${pop}.bed"),
          file("$dir/${pop}.bim"),
          file("$dir/${pop}.fam")]
    }
    .set { plink_data }

plink_data.subscribe { println "$it" }
```

```
[data/pops/YRI.bed, data/pops/YRI.bim, data/pops/YRI.fam]
[data/pops/CEU.bed, data/pops/CEU.bim, data/pops/CEU.fam]
[data/pops/BEB.bed, data/pops/BEB.bim, data/pops/BEB.fam]
```

Grouped Files - Version 1: map

```
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params.dir = "data/pops/"
dir = params.dir
params.pops = ["YRI","CEU","BEB"]

Channel
    .from(params.pops)
    .map { pop ->
        [ file("$dir/${pop}.bed"),
          file("$dir/${pop}.bim"),
          file("$dir/${pop}.fam")]
    }
    .set { plink_data }

plink_data.subscribe { println "$it" }
```

```
process getFreq {
  input:
  tuple path(bed), path(bim), path(fam)

  output:
  path("${bed.baseName}.frq"), emit result

  """
  plink --bed $bed \
    --bim $bim \
    --fam $fam \
    --freq \
    --out ${bed.baseName}"
  """
}

workflow {
  getFreq(plink_data).view()
}
```

```
[data/pops/YRI.bed, data/pops/YRI.bim, data/pops/YRI.fam]
[data/pops/CEU.bed, data/pops/CEU.bim, data/pops/CEU.fam]
[data/pops/BEB.bed, data/pops/BEB.bim, data/pops/BEB.fam]
```

Grouped Files - Version 2: `fromFilePairs`

Use `fromFilePairs`.

- Takes a closure used to gather files together with the same key

```
x_ch = Channel.fromFilePairs( files ) { closure }
```

- Specify the files as a glob
- Closure associates each file with a key
- `fromPairs` puts all files with same key together
- Returns a list of pairs (key, list)

Grouped Files - Version 2: `fromFilePairs`

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```

- Specify the files as a glob
- Closure associates each file with a key
- `fromPairs` puts all files with same key together
- Returns a list of pairs (key, list)

```
#!/usr/bin/env nextflow

commands = Channel.fromFilePairs("/usr/bin/*", size:-1) {
                it.baseName[0]
           }

commands.subscribe { k= it[0];
  n=it[1].size();
  println "There are $n files starting with $k";
}
```

A more complex example – default closure

```
Channel
    .fromFilePairs
        ("${params.dir}/*.{bed,fam,bim}",size:3, flat : true)
    .ifEmpty { error "No matching plink files" }
    .set { plink_data }

plink_data.subscribe { println "$it" }
```

Grouped Files - Version 2: `fromFilePairs`

Use `fromFilePairs`.

- Takes a closure used to gather files together with the same key

```
x_ch = Channel.fromFilePairs( files ) { closure }
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```
#!/usr/bin/env nextflow

commands = Channel.fromFilePairs("/usr/bin/*", size:-1) {
                it.baseName[0]
           }

commands.subscribe { k= it[0];
  n=it[1].size();
  println "There are $n files starting with $k";
}
```

A more complex example – default closure

```
Channel
    .fromFilePairs
        ("${params.dir}/*.{bed,fam,bim}",size:3, flat : true)
    .ifEmpty { error "No matching plink files" }
    .set { plink_data }

plink_data.subscribe { println "$it" }
```

```
[CEU, [data/pops/CEU.bed, data/pops/CEU.bim, data/pops/CEU.fam]]
[YRI, [data/pops/YRI.bed, data/pops/YRI.bim, data/pops/YRI.fam]]
[BEB, [data/pops/BEB.bed, data/pops/BEB.bim, data/pops/BEB.fam]]
```

Grouped Files - Version 2: `fromFilePairs`

```
process checkData {
    input:
    tuple val(pop), path(pl_files)

    output:
    path("${pl_files[0]}.frq"), emit: result

    """
    plink --bfile $base --freq --out pl_files[0].baseName
    """
}
```

Grouped Files - Version 2: `fromFilePairs`

```
process checkData {
    input:
    tuple val(pop), path(pl_files)

    output:
    path("${pl_files[0]}.frq"), emit: result

    """
    plink --bfile $base --freq --out pl_files[0].baseName
    """
}
```

```
process checkData {
    input:
    tuple val(pop), path(pl_files)

    output:
    path("${pop}.frq"), emit: result

    """
    plink --bfile $pop --freq  --out $pop
    """
}
```

Grouped Files - Final Version

```
#!/usr/bin/env nextflow
nextflow.enable.dsl=2

params.dir = "data/pops/"
dir = params.dir
params.pops = ["YRI","CEU","BEB"]

Channel
    .fromFilePairs("${params.dir}/{YRI,BEB,CEU}.{bed,bim,fam}",size:3) {
        file -> file.baseName
    }
    .filter { key, files -> key in params.pops }
    .set { plink_data }

process checkData {
    input:
    tuple val(pop), path(pl_files)

    output:
    path("${pop}.frq"), emit: result

    """
    plink --bfile $pop --freq  --out $pop
    """

workflow {
  checkData(plink_data).view()
}
```

Exercise 5

Have a look at ex5-weather.nf. In the data directory are set of data files for different years and months. First, I want you to use paste to combine all the files for the same year and month (paste joins files horizontal-wise). Then these new files should be concated.

Generalising and Extending

On absolute paths

Absolute paths

```
input = Channel.fromPath("/data/batch1/myfile.fa")

process show {
    input:
    path(data)

    output:
    path('see.out')

    """
    cp ${data} /home/scott/answer
    """
    ...
```

Nextflow and Docker

Nextflow and Docker

Docker & Singularity Containers

Docker & Singularity Containers

Light-weight virtualisation abstraction layer

- Currently runs on Unix like systems
    - Linux
    - macOS
- Windows support coming

Can create images locally or get from repositories

```
## Docker
docker pull ubuntu
docker pull quay.io/banshee1221/h3agwas-plink

## Singularity
singularity pull docker://ubuntu
singularity pull docker://quay.io/banshee1221/h3agwas-plink
```

Running images

```
## Docker
docker run <some-image-name>

## Singularity
singularity exec <some-image-name>
```

- Docker/Singularity often run images in background
- Can also run interactively

```
## Running Docker interactively
sudo docker run -t -i quay.io/banshee1221/h3agwas-plink

## Running Singularity interactively
singularity shell docker://quay.io/banshee1221/h3agwas-plink
```

Nextflow supports Docker & Singularity

- Well designed script should be highly portable
- Each process gets run as a separate image call
    - Under the hood, a **`docker run`** or a **`singularity exec`** is called
- Can use the same or different images for each process
    - Parameterisable

Assuming all processes use the same image:

```
## For Docker
nextflow run plink2.nf -with-docker quay.io/banshee1221/h3agwas-plink

## For Singularity
nextflow run plink.nf -with-singularity docker://quay.io/banshee1221/h3agwas-plink
```

Nextflow and Docker

Directory & File Access

Directory & File access

Nextflow Docker/Singularity support highly transparent – but pay attention to good practice

- For each process Docker/Singularity mounts the work directory for **that** process on the Docker/Singularity image.
- Files can be staged in and out using Nextflow mechanisms.
- Other files available: directories mounted through Docker/Singularity run time options or on the Docker image
- No other files on the host machine including the current directory
- Process executes in the Docker/Singularity environment

Directory & File access

```
#!/usr/bin/env nextflow
nextflow.enable.dsl=2

data = Channel.fromPath("data/pops/YRI.bim")

process see {
    publishDir "count_out", overwrite:true, mode:'move'
    echo true

    input:
    path(bim)

    output:
    path(count)

    """
    hostname
    echo "Path is \$( pwd )\n "
    echo "Parent directory has \$( ls .. )\n"
    echo "My home directory has \$( ls /home/phele )\n"
    wc -l ${bim} > count
    ls
    """
}

workflow {
    see(data)
}
```

```
N E X T F L O W  ~  version 0.21.2
Launching show_env.nf
[warm up] executor > local
[94/597f09] Submitted process > see (1)
89ad448ae0b2
Path is /home/scott/witsGWAS/dockerized/work/94/597f09ca6cc01c7be
Parent directory has 597f09ca6cc01c7be
My home directory has witsGWAS

YRI.bim
count
```

Directory & File access

Note that although the script's pwd shows:
`/home/scott/witsGWAS/dockerized/work/94/597f09ca6cc01c7be`

- Only these specific directories are mounted
- Only the files in the innermost directory are available

Any absolute paths (other than those used in staging) will result in error.

Profiles

In nextflow.config

```
profiles {
  ...
  docker {
    process.container = 'quay.io/banshee1221/h3agwas-plink:latest'
    docker.enabled = true
  }
}
```

Now can run as:

```
nextflow run gwas.nf -profile docker
```

This can be extended in many ways

- Different processes can use different containers
- Can mount other host directories
- Can pass arbitrary Docker parameters

Executors

Executors

Executors

Executors

A Nextflow *executor* is the mechanism which Nexflow runs the code in each of the processes

- Default is `local`: process is run as a script

Many others

- PBS/Torque
- SLURM
- Amazon (AWS Batch)
- SGE (Sun Grid Engine)

Selecting an executor Annotating each process

- `executor` directive, e.g. `executor 'pbs'`
- resource constraints

Or, `nextflow.config` file

- either global or per-process

Executors

Nextflow on a cluster (HPC)

Running Nextflow on a cluster (HPC)

Script runs on the *head* node

- Nextflow uses the **`executor`** information to decide how the job should run
- Each process can be handled differently
- Nextflow submits each process to the job scheduler on your behalf (e.g, if using PBS/Torque, **`qsub`** is done)

Example

```
process {
  executor = 'pbs'
  queue = 'batch'
  scratch = true
  cpus = 5
  memory = '2GB'
}
```

Executors

Scheduler + Docker

Scheduler + Docker

```
process.container = 'quay.io/banshee1221/h3agwas-plink:latest'
docker.enabled = false

process {
  executor = 'pbs'
  queue = 'batch'
  scratch = true
  cpus = 5
  memory = '2GB'
}
```

Executors

Amazon EC2

Amazon EC2

Netflow has native support for EC2

- You need an account on EC2
- Image (AMI) with the appropriate support

Launch your code:

```
nextflow cloud create GenomeCloud -c 5
```

If successful, Nextflow will give you the name of the headnode of your cluster

- `ssh` into into it
- run Nextflow on it.

Afterwards shut down:

```
nextflow shutdown GenomeCloud
```

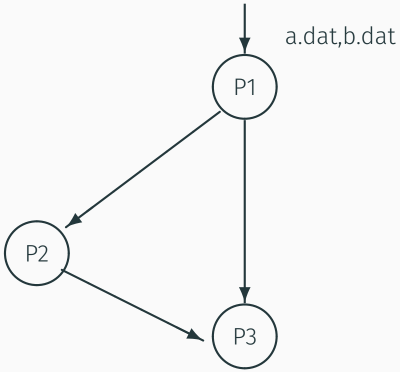
Channel Operations

Channel operations

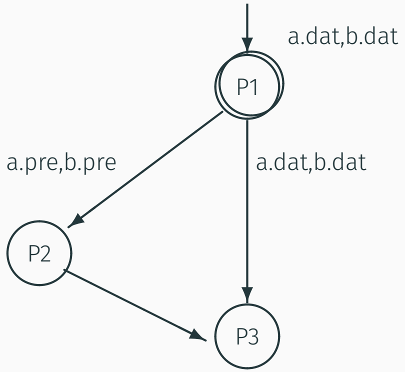
Nextflow tries to maximise concurrency

- processes are by default synchronised by channels
- when data arrives on all input channels, process executes

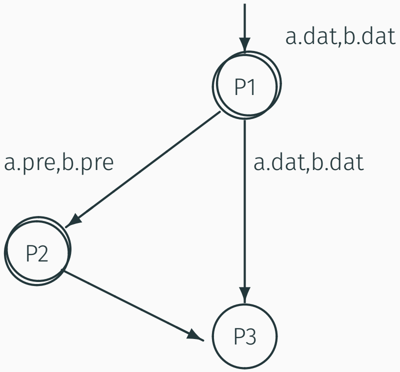
Channel operations



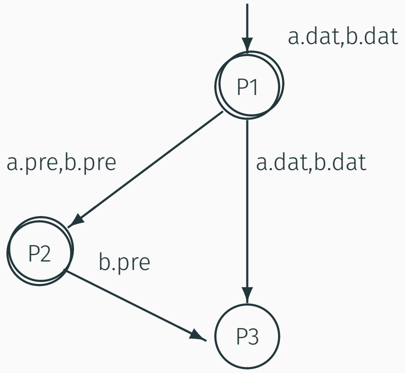
Channel operations



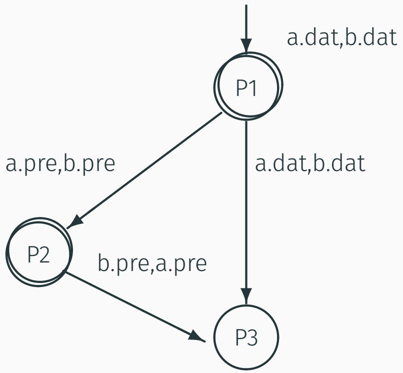
Channel operations



Channel operations



Channel operations



Channel operations

```
#!/usr/bin/env nextflow
nextflow.enable.dsl=2

Channel.fromPath("/home/phelelani/*.dat").set { data }

process P1 {
    input:
    path(data)

    output:
    path("${data.baseName}.pre"), emit: channelA
    path(data), emit: channelB

    """
    echo dummy > ${data.baseName}.pre
    """
}

process P2 {
    input:
    path(channelA)

    output:
    path(channelA), emit: channelC

    """
    if [ ${channelA.baseName} = "a" ]
    then
        echo ${channelA.baseName}
        sleep 4
```

Channel operations

```
#!/usr/bin/env nextflow
nextflow.enable.dsl=2

Channel.fromPath("/home/phelelani/*.dat").set { data }

process P1 {
    input:
    path(data)

    output:
    path("${data.baseName}.pre"), emit: channelA
    path(data), emit: channelB

    """
    echo dummy > ${data.baseName}.pre
    """
}

process P2 {
    input:
    path(channelA)

    output:
    path(channelA), emit: channelC

    """
    if [ ${channelA.baseName} = "a" ]
    then
        echo ${channelA.baseName}
        sleep 4
    else
        echo ${channelA.baseName}
        sleep 1
    fi
    """
}

process P3 {
    echo true

    input:
    path(channelB)
    path(channelC)

    script:
    """
    echo "${channelB} - ${channelC}"
    """
}

workflow {
    P1(data)
    P2(P1.out.channelA).view()
    P3(P1.out.channelB, P2.out.channelC)
}
```

Channel operations

Solution: `join`/`merge` channels

- `x.merge(y)`
  Items emmited by the channels *x* and *y* are combined into a new channel.
- `x.join(y)`
  Items emmited by the channels *x* and *y* are joined together into one channel based on existing matching key. Default: first element in each item.

Channel Operations

Using `join`

Using join

```
ch1 = Channel.from( "a","b","c" )
ch2 = Channel.from( "a","d","e","a","c","b" )
ch1.join(ch2).subscribe { println it }
```

```
a
b
c
```

Using join

```
ch1 = Channel.from( "a","b","c" )
ch2 = Channel.from( "a","d","e","a","c","b" )
ch1.join(ch2).subscribe { println it }
```

```
a
b
c
```

Tuples:

```
ch1 = Channel.from( ["a",1], ["b",4], ["c",5] )
ch2 = Channel.from( ["a",10], ["d",8], ["e",7], ["a",9], ["c",1], ["b",10] )
ch1.merge(ch2).subscribe { println it }
```

```
[a, 1, 10]
[b, 4, 10]
[c, 5, 1]
```

Channel Operations

Using `merge`

Using merge

```
ch1 = Channel.from( "a","b","c" )
ch2 = Channel.from( "a","d","e","a","c","b" )
ch1.merge(ch2).subscribe { println it }
```

```
[a, a]
[b, d]
[c, e]
```

Using merge

```
ch1 = Channel.from( "a","b","c" )
ch2 = Channel.from( "a","d","e","a","c","b" )
ch1.merge(ch2).subscribe { println it }
```

```
[a, a]
[b, d]
[c, e]
```

Tuples:

```
ch1 = Channel.from( ["a",1], ["b",4], ["c",5] )
ch2 = Channel.from( ["a",10], ["d",8], ["e",7], ["a",9], ["c",1], ["b",10] )
ch1.merge(ch2).subscribe { println it }
```

```
[a, 1, a, 10]
[b, 4, d, 8]
[c, 5, e, 7]
```

Channel Operations

`join` vs `merge`

`join` vs `merge`

`join`

- If values are singletons, then the values must be the same
- If value is tuple if the, then the first element of the tuple must be the same

`merge`

- Merges everything into a channel, no matching.

Channel Operations

Working version of the example

Working version of the example

```
Channel.fromPath(""/home/phelelani/*.dat").set { data }

process P1 {
    echo true

    input:
    file(data)

    output:
    set val(data.baseName), file("${fbase}.pre") into channelA
    set val(data.baseName), file(data) into channelB

    script:
    fbase=data.baseName
    "echo dummy > ${fbase}.pre"

process P2 {
    echo true

    input:
    set name, file(pre) from channelA

    output:
    set name, file(pre) into channelC

    script:
    if (pre.baseName = /.*TMP.*/)
      "sleep 4"
    else
      "sleep 1"
}

process P3 {
    echo true

    input:
    set name, file(data), file(pre) from channelB.join(channelC)

    script:
    """
    echo "${data} - ${pre}"
    """
}
```

Channel Operations

Copying channels

Copying channels

You often need to copy a channel

```
process do {
    ..

    output:
    file ("x.*") into out_ch

    ..
}

out_ch.separate(a_ch, b_ch, c_ch)
```

Copying channels

You often need to copy a channel

```
process do {
    ..

    output:
    file ("x.*") into out_ch

    ..
}

out_ch.separate(a_ch, b_ch, c_ch)
```

Alternatively

```
process do {
    ..

    output:
    file ("x.*") into (a_ch, b_ch, c_ch)

    ..
}
```