

Bioinformatics session

3rd Annual workshop on
bioinformatics and variant
interpretation in InPreD

https://inpred.github.io/25-06_bioinfo_ws/bioinfo_ws



1. Unit testing

What is unit testing?

- test smallest piece of code that can be logically isolated in software application (function, subroutine, method)
- the smaller the better - more granular view of what is going on; also faster
- should not cross systems (database, filesystem, network) -> integration and functional tests

Example

```
# calculator.py
def add(x, y):
    """add numbers"""
    return x + y
```

```
# test_calculator.py
import calculator

def test_add():
    assert calculator.add(1, 2) == 3
```

Why do we need unit testing?

- early defect detection
- code quality improvement
- facilitates refactoring
- faster development cycles
- better documentation
- enables more frequent releases

How to design a unit test?

- identify the unit (function, method)
- what is its functionality?
- what is the input (correct and incorrect)?
- how to handle incorrect input? (edge cases, invalid data)
- what does it return?
- positive and negative results should be tested

Set up unit testing for your functions

- install pytest

```
$ pip install pytest
```

- add your function to a module at `my_module/my_module.py`
- add your unit test at `my_module/tests/my_module_test.py`
- in the test file import your module `from my_module.my_module import my_function`

First exercise

- go to https://github.com/InPreD/25-06_bioinfo_ws_unit_testing

25-06_bioinfo_ws_unit_testing Public

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main 1 Branch 0 Tags

Go to file

Add file <> Code

marrip fix: rm proxy

.devcontainer fix: rm proxy

LICENSE Initial commit

README.md Initial commit

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25-06_bioinfo_ws_unit_testing

codespace template for unit testing workshop

Local Codespaces

Codespaces

Your workspaces in the cloud

On current branch

shiny space eureka 3d

main No changes

Create a codespace on main

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Languages

Dockerfile 100.0%

Suggested workflows

Based on your tech stack

First exercise

← →

25-06_bioinfo_ws_unit_testing [Codespaces: shiny space eureka]

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EXPLORER

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25-06_BIOINFO_WS_UNIT_TESTING [CODESPA...

> .devcontainer

🔑 LICENSE

📘 README.md

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> GLIEDERUNG

> ZEITACHSE

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PROBLEME

AUSGABE

DEBUGGING-KONSOLE

TERMINAL

PORTS

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```
root@codespaces-defab7:/workspaces/25-06_bioinfo_ws_unit_testing#
```

>< Codespaces: shiny space eureka

🔗 main ↺

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👤 Layout: German

🔔

First exercise

- pytest was already installed in the codespace
- the suggested layout was already applied
- create a branch for your work:

```
$ git checkout -b unit-tests-<your name>
```

- start with the first exercise in `first/tests/first_test.py`
- whenever you are done, commit your changes (use [commit message conventions](#)):

```
$ git add first/tests/first_test.py  
$ git commit -m "test: <your commit message>"
```

- and we push them to GitHub:

```
$ git push --set-upstream origin unit-tests-<your name>
```

Handle exceptions in unit tests

- functions can raise exceptions and we would like to test for those
- import `pytest` to have access to `raises()`
- add `with` -block to handle the exception:

```
import calculator
import pytest

def test_add_exception():
    with pytest.raises(TypeError):
        assert add("one", "two") == None
```

Second exercise

- continue with the second exercise in `second/tests/second_test.py`
- whenever you are done, commit your changes (use [commit message conventions](#)):

```
$ git add second/tests/second_test.py  
$ git commit -m "test: <your commit message>"
```

- and we push them to GitHub:

```
$ git push
```

Make unit tests table-driven by using parametrize

- having more than one test case results in repeating a lot of code (one function per test case)
- to condense this as much as possible (ideally one unit test per function), we can use the `pytest` decorator `parametrize`
- again, import `pytest` to gain access to the decorator
- add the decorator `@pytest.mark.parametrize` as a header to your function
- define the required variables (input, exception, output)
- add your test cases as a list of tuples (one tuple per case)
- also use `nullcontext` from the module `contextlib` to account for cases without exceptions

```
import calculator
import pytest

from contextlib import nullcontext

@pytest.mark.parametrize(
    "x, y, exception, want",
    [
        (1, 2, nullcontext(), 3),
        ("one", "two", pytest.raises(TypeError), None)
    ]
)
def test_add(x, y, exception, want):
    with exception:
        assert add(x, y) == want
```

Third exercise

- continue with the third exercise in `third/tests/third_test.py`
- whenever you are done, commit your changes (use [commit message conventions](#)):

```
$ git add third/tests/third_test.py  
$ git commit -m "test: <your commit message>"
```

- and we push them to GitHub:

```
$ git push
```

Use GitHub action to automatically run tests on push

- add `.github/workflows/main.yml` :

```
name: Python test
on: push

jobs:
  test:
    name: Run unit tests
    runs-on: ubuntu-latest
    steps:
      -
        name: Check out the repo
        uses: actions/checkout@v4
      -
        name: Set up Python 3.12.8
        uses: actions/setup-python@v4
        with:
          python-version: 3.12.8
      -
        name: Install dependencies
        run: pip install -r requirements.txt
      -
        name: Unit testing
        uses: pavelzw/pytest-action@v2
        with:
          verbose: true
          emoji: true
          job-summary: true
          custom-arguments: -q
          click-to-expand: true
          report-title: 'Bioinfo workshop unit testing'
```


Use GitHub action to automatically run tests on push

- if you don't want to write all of that, merge the branch containing the file into your branch:

```
$ git merge add-github-action
```

Fourth exercise

- write unit tests for the functions in `fourth/fourth.py`
- whenever you are done, commit your changes (use [commit message conventions](#)):

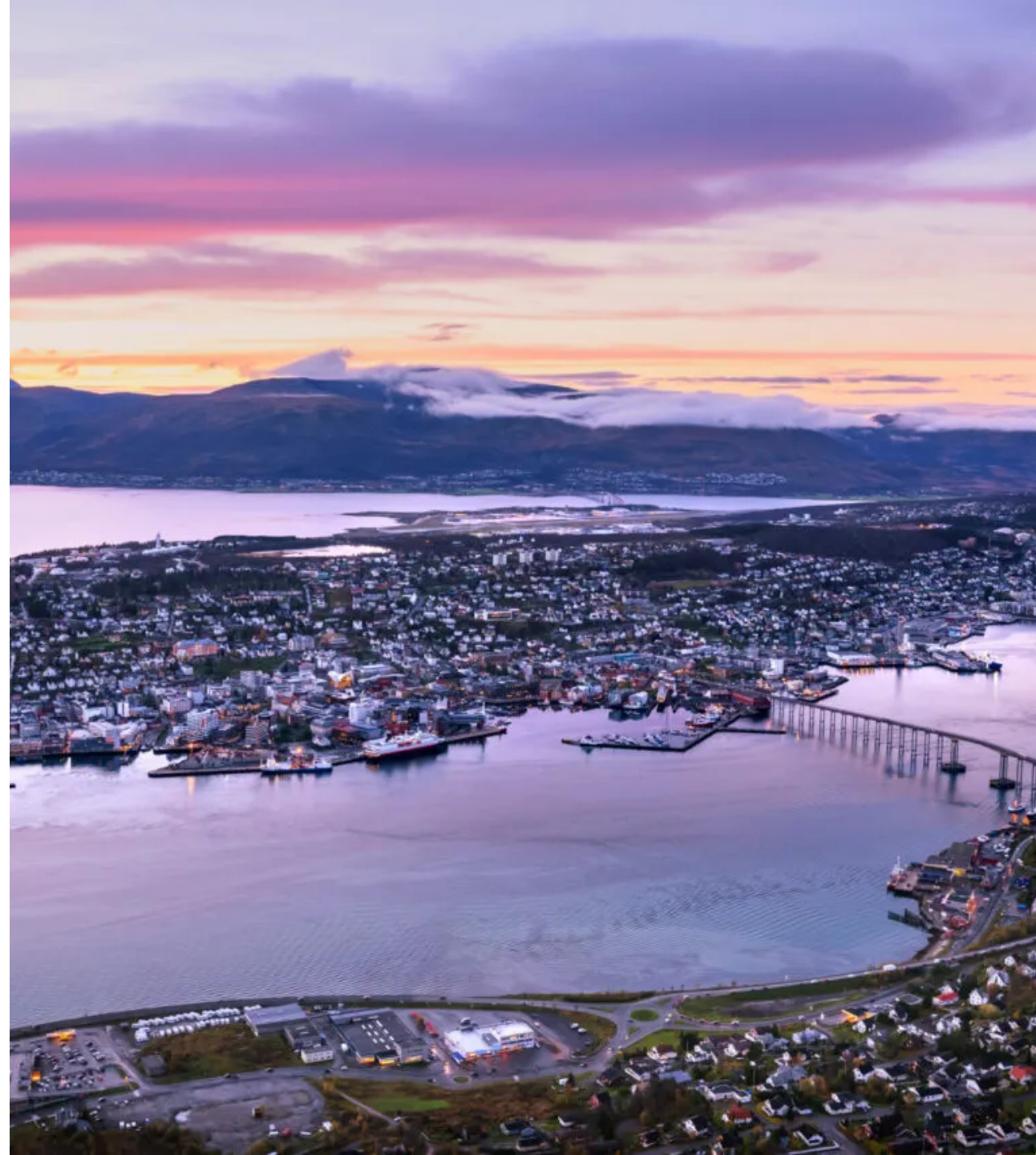
```
$ git add third/tests/third_test.py  
$ git commit -m "test: <your commit message>"
```

- and we push them to GitHub:

```
$ git push
```

Thank you for your attention!

Day 1 done!



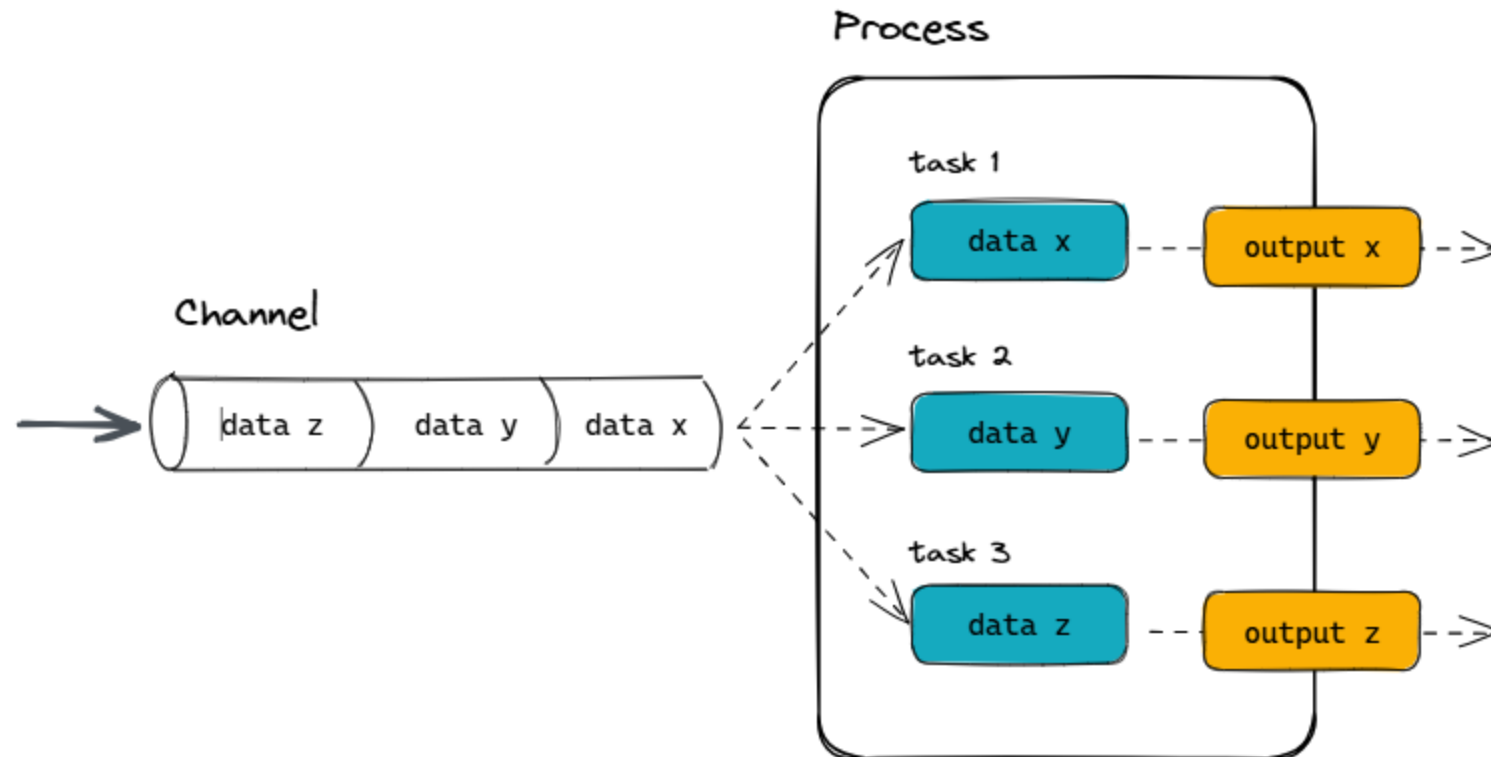
2. Nextflow

What is nextflow?

- workflow orchestration engine, domain-specific language (in contrast to general-purpose language, e.g. python)
- easy to write data-intensive computational workflows
- extension of groovy which is a superset of Java
- core features:
 - portability and reproducibility
 - scalability of parallelization and deployment
 - integration of existing tools, systems, and industry standards

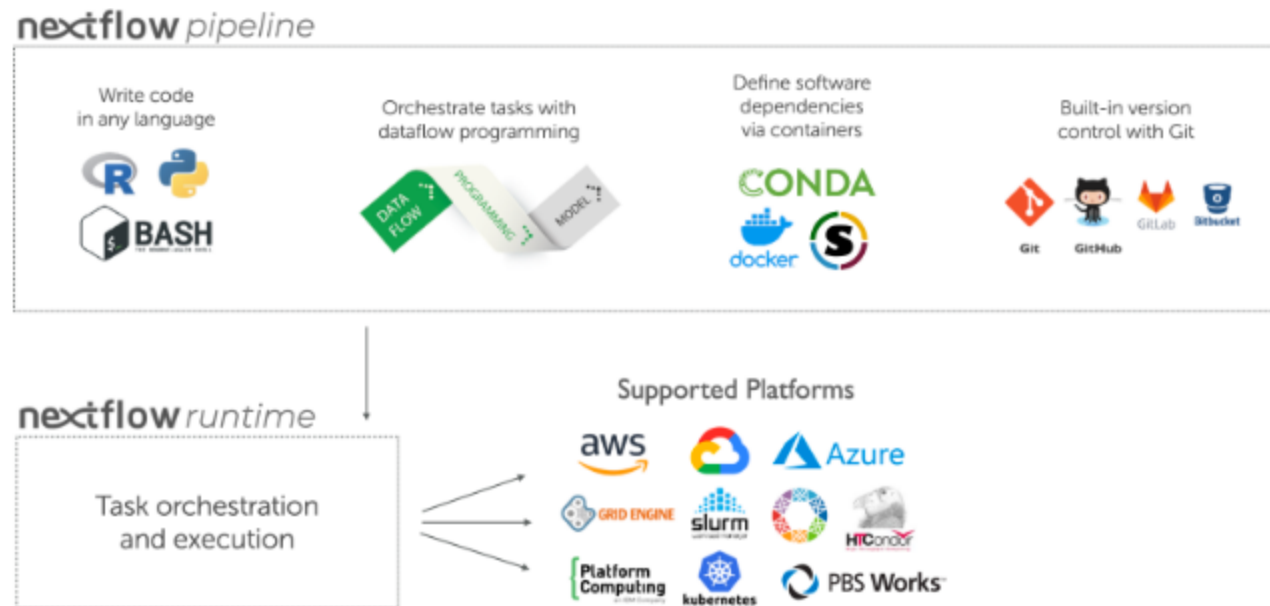
Processes and channels

- different processes joined together - each written in any language that can be executed by Linux platform
- independently and isolated processes - not sharing common (writable) state
- communication via asynchronous first-in, first-out (FIFO) queues, called `channels`



Execution abstraction

- process = *what* is executed <-> executor = *how* it is executed
- provides abstraction between workflow's functional logic and underlying execution system/runtime
- workflow runs seamlessly on local computer, HPC cluster or cloud



Let's get started

- go to https://github.com/InPreD/25-06_bioinfo_ws_nextflow

25-06_bioinfo_ws_nextflow Public

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main 1 Branch 0 Tags

Go to file

Add file <> Code

Local Codespaces

Codespaces Your workspaces in the cloud

Create a codespace on main

On current branch

miniature fishstick 1h

main* Uncommitted changes

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Suggested workflows

Based on your tech stack

- create a branch for your work

```
$ git checkout -b nextflow-<your name>
```

- create a new file `hello_world.nf`
- write a workflow which outputs a file containing "Hello World!"

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

/*
 * Use echo to print 'Hello World!' to a file
 */
process sayHello {

    output:
        path 'output.txt'

    script:
        """
        echo 'Hello World!' > output.txt
        """
}

workflow {

    // emit a greeting
    sayHello()
}
```

- try to run it

```
$ nextflow run hello_world.nf
```

```
root@52abc3ecdd95 /w/25-06_bioinfo_ws_nextflow (main)# nextflow run hello_world.nf
Nextflow 25.04.1 is available - Please consider updating your version to it

NEXTFLOW ~ version 24.10.4

Launching `hello_world.nf` [boring_rubens] DSL2 - revision: 595ea09581

executor > local (1)
[33/7106de] process > sayHello [100%] 1 of 1 ✓
```

- check if you can find `work/33/7106de/output.txt`
- explore the other files that are in `work/33/7106de/`

- add a directory to which results should be published

```
process sayHello {  
    publishDir 'results', mode: 'copy'  
    output:  
        path 'output.txt'  
    ...  
}
```

- add a greeting variable

```
process sayHello {  
    publishDir 'results', mode: 'copy'  
  
    input:  
        val greeting  
  
    output:  
        path 'output.txt'  
  
    script:  
        """  
        echo '$greeting' > output.txt  
        """  
}  
  
workflow {  
    // emit a greeting  
    sayHello(params.greeting)  
}
```

```
$ nextflow run hello_world.nf --greeting 'Heisann!'
```

- move the `params.greeting` into the `hello_world.nf` :

```
params.greeting = 'Heisann!'

process sayHello {
    publishDir 'results', mode: 'copy'
    ...
}
```

```
$ nextflow run hello_world.nf
```

```
$ nextflow run hello_world.nf --greeting 'Hejsan!'
```

- transform greetings into a channel

```
process sayHello {  
    input:  
        val greeting  
  
    output:  
        stdout  
  
    script:  
    """  
    echo '$greeting'  
    """  
}  
  
workflow {  
    greeting_ch = Channel.of('Alo', 'Salut', 'Sunt eu').view()  
    // emit a greeting  
    sayHello(greeting_ch) | view  
}
```

```
$ nextflow run hello_world.nf -ansi-log false # run it several times
```

Channels

- processes communicate through channels
- two major properties:
 - Sending a message is an asynchronous (i.e. non-blocking) operation
 - Receiving a message is a synchronous (i.e. blocking) operation
- please refer to the [nextflow docs about channels](#)

- create a `.csv` file containing our greetings which will serve as input

```
Alo  
Salut  
Sunt eu
```

- create channel from the file using the channel factory `fromPath()`

```
workflow {  
  
    greeting_ch = Channel.fromPath(params.greeting).view()  
    // emit a greeting  
    sayHello(greeting_ch) | view  
}
```

```
$ nextflow run hello_world.nf -ansi-log false --greeting greetings.csv
```

- try to manipulate a channel by using the operators `splitCsv()` and `map()`

```
workflow {  
    greeting_ch = Channel.fromPath(params.greeting)  
        .view( it -> "Before splitCsv: $it" )  
        .splitCsv()  
        .view( it -> "After splitCsv: $it" )  
        .map( item -> item[0] )  
        .view( it -> "After map: $it" )  
    // emit a greeting  
    sayHello(greeting_ch) | view  
}
```

```
$ nextflow run hello_world.nf -ansi-log false --greeting greetings.csv
```

- please refer to the [nextflow docs about channel operators](#)

- add a second process

```
process convertToUpper {  
    input:  
        path lower  
  
    output:  
        lower  
  
    script:  
    """  
    echo '$lower' | tr '[a-z]' '[A-Z]'  
    """  
}
```

- include the process in the workflow and link it to the first one

```
workflow {  
  
    greeting_ch = Channel.fromPath(params.greeting)  
        .view( it -> "Before splitCsv: $it" )  
        .splitCsv()  
        .view( it -> "After splitCsv: $it" )  
        .map( item -> item[0] )  
        .view( it -> "After map: $it" )  
  
    // emit a greeting  
    sayHello(greeting_ch) | view  
    convertToUpper(sayHello.out) | view  
}
```

```
$ nextflow run hello_world.nf -ansi-log false --greeting greetings.csv
```