DiFlow



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Introduction

DiFlow¹ is an abstraction layer on top of NextFlow²'s DSL2³. DiFlow is a set of principles and guidelines for building NextFlow pipelines that allow the developer to declaratively define processing components and the user to declare the pipeline logic in a clean and intuitive way.

Viash⁴ is a tool that (among other things) allows us to *use* DiFlow and make it practical, without the burden of maintaining boilerplate or *glue* code.

Functional Reactive Programming (FRP)

If you're new to Functional Reactive Programming (FRP), here are a few pointers to posts and a video that introduce the concepts:

- An excellent Medium post⁵ from Timo Stöttner
- The introduction⁶ to Reactive Programming you've been missing from André Staltz.
- A very insightful presentation by Staltz where he introduces FRP from first principles (with live coding).

In what follows, we will refer to *streams* in line with those authors but if you're used to working with Rx⁸ you would call this an observable.

FRP for pipelines

Other initiatives have recognized that FRP is a good fit for pipeline development. Recent research and development also confirms this:

- Skitter⁹
- Krews¹⁰

¹ https://pointer

² https://www.nextflow.io/

³ https://www.nextflow.io/docs /latest/dsl2.html

 $^{^4}$ http://data-intuitive.com/vias h_docs

⁵ https://itnext.io/demystifying-functional-reactive-programmin g-67767dbe520b

⁶ https://gist.github.com/staltz /868e7e9bc2a7b8c1f754

⁷ https://www.youtube.com/wa tch?v=fdol03pcvMA

⁸ http://reactivex.io/

⁹ https://soft.vub.ac.be/~math saey/skitter/

¹⁰ https://github.com/weng-lab/krews

NextFlow

Introduction

For a step-by-step introduction to NextFlow (both the original DSL as well as DSL2), please refer to this repository 11 created and maintained by the VIB 12 .

Another very interesting resource is this cheatsheet¹³ by Daniele Cook. It not only contains a handy cheat sheet, but also some conventions one should know about as well as some pitfalls.

FRP in NextFlow

The c_{hannel}^{14} class used by NextFlow, itself based on the DataFlow Programming $Model^{15}$ can in fact be regarded as an implementation of a Functional Reactive Programming library. Having said that, NextFlow allows one to to mix functional and imperative programming to the point that a developer is able to shoot its own foot.

Furthermore, Channels can not be nested which complicates certain operations on the streams.

NextFlow DSL(2)

 ${
m DSL2^{16}}$ is a crucial development in NextFlow because it avoid having to maintain large, monolithic pipeline definitions in one file. With DSL2, developer can spin off functionality in separate files and <code>import</code> what is needed.

This also potentially opens up ways to build (reusable) modules that could be used in different projects. That is exactly what a lot of organizations need.

https://github.com/vibbits/n extflow-course

¹² https://vib.be/

¹³ https://github.com/danrlu/ Nextflow_cheatsheet

https://www.nextflow.io/docs /latest/channel.html

https://en.wikipedia.org/wiki/Dataflow_programming

https://www.nextflow.io/docs /latest/dsl2.html

DiFlow

The NoPipeline approach

For developing the pipeline, we set out with a few goals in mind:

- Build modules where each modules deals with a specific (computational) task
- Make sure those modules can be reused
- Make sure the module functionality can be tested and validated
- Make sure modules have a consistent API, so that
 - a. calling a module is straightforward
 - b. including a module in a pipeline is transparent and seamless

Please note that nothing in these requirements has to do with running a pipeline itself. Rather, we consider this a bottom-up system whereby we first focus on a solid foundation before we actually start to tie things together.

That's why we call this the NoPipeline approach, similar to NoSQL where 'No' does not stand for *not*, but rather 'Not Only'. The idea is to focus on the pipeline aspect *after* the steps are properly defined and tested.

General Requirements and design principles

Reproducibility

I originally did not include it as a design principle for the simple reason that I think it's obvious. This should be every researcher's top priority.

Pipeline Parameters vs Runtime Parameters

We make a strict distinction between parameters that are defined for the *FULL* pipeline and those that are defined at runtime.

Pipeline Parameters We currently have 4 pipeline parameters: Docker prefix, ddir, rdir and pdir.

Runtime Parameters Runtime parameters differ from pipeline parameters in that they may be different for parallel runs of a process. A few examples:

- Some samples may require different filter threshold than others
- After concatenation, clustering may be run with different cluster parameters

• etc.

In other words, it does not make sense to define those parameters for the full pipeline because they are not static.

Consistent API

When we started out with the project and chose to use NextFlow as a workflow engine, I kept on thinking that the level of abstraction should have been higher. With DSL1, all you could do was create one long list of NextFlow code, tied together by Channels.

With DSL2, it became feasible to *organise* stuff in separate NextFlow files and import what is required. But in larger codebases, this is not really a benefit because every modules/workflow may have its own parameters and output. No structure is imposed. Workflows are basically functions taking parameters in and returning values.

I think it makes sense to define an API and to stick to it as much as possible. This makes using the modules/workflows easier...

Flat Module Structure

We want to avoid having nested modules, but rather support a pool of modules to be mixed and matched.

As a consequence, this allows a very low threshold for including third-party modules: just add it to the collection of modules and import it in the pipeline. In order to facilitate the inclusion of such third-party modules that are developed in their own respective repositories, we added one additional layer in the hierarchy allowing for such a splitting.

Job Serialization

We avoid requiring the sources of the job available in the runtime environment, i.e., the Docker container. In other words, all code and config is serialized and sent with the *process*.

An abstract computation step

The module concept inspired us to think of an abstract way to represent a computation step and implement this in NextFlow. We wrote [Portash] to this end. But Portash had its shortcomings. The most important of which was that it did not adhere to separation of concerns: execution definition (what?) where mixed up with execution context (how?/where?). Moreover, dynamic nature of Portash lends itself well to running a tool as a service, but not so much in a batch process.

Nevertheless, we were able to express a generic NextFlow step as pure *configuration* that is passed to a process at runtime. This allows for some very interesting functionality. Some prototypes were developed, the last one of which could run a single-cell RNA pipeline from mapping to generating an integrated dataset combining different samples.

The run-configuration was provided by means of a Portash YAML spec residing in the module directory. It must be stressed that not requiring the component *code* to be already available inside the container is a big plus. It means a container contains dependencies, not the actual run script so the latter can be updated more frequently. This is especially useful during component and pipeline development.

Our first implementation had a few disadvantages:

- It contained a mix of what to run and how to run it, but it did not contain information on the container to run in. This had to be configured externally, but then the module is not an independent entity anymore.
- Specifying and overriding YAML content in Groovy is possible, but not something that is intuitive. We worked around that by letting the user specify custom configuration using a Groovy nested Map.
- The module functionality was abstracted with a consistent API and the difference between 2 modules was just a few lines of code with a different name or pointer. But still, one had to maintain that and making a similar change in a growing set of module files is a recipe for mistakes.

But overall, the concept of an abstract computation step proved to work, it was just that a few ingredients were still missing it seemed. On the positive side, we showed that it's possible to have an abstract API for (NextFlow) modules that keeps the underlying implementation hidden while improving the readability of the pipeline code.

Toward implementation

What is needed as information in order to run a computation step in a pipeline?

- 1. First, we need data or generally speaking, **input**. Components/modules and pipelines should run zero-touch, so input has to be provided at startup time.
- 2. Secondly, we need to know what to run en how to run it. This is in effect the definition of a modules or pipeline step.
- 3. Thirdly, in many cases we will require the possibility to change parameters for individual modules in the pipeline, for instance cutoff values for a filter, or the number of clusters for a clustering algorithm. The classical way to do that is via the params object.

One might wonder if there is a difference between input and parameters pointing to input is also a kind of parametrization. The reason those are kept apart is that additional validation steps are necessary for the data. Most pipeline systems trace input/output closely whereas parameters are ways to configure the steps in the pipeline.

In terms of FRP, and especially in the DataFlow model, we also have to keep track of the *forks* in a parallel execution scenario. For instance, if 10 batches of data can be processed in parallel we should give all 10 of them an ID so that individual forks can be distinguished. We will see that those IDs become crucial in most pipelines.

We end up with a model for a stream/channel as follows (conceptually):

```
[ ID, data, config ]
```

were

- ID is just a string or any object for that matter that can be compared later. We usually work with strings.
- data is a pointer to the (input) data. With NextFlow, this should be a Path object, ideally created using the file() helper function.
- config is a nested Map where the first level keys are chosen to be simply an identifier of the pipeline step. Other approaches can be taken here, but that's what we did.

This can be a triplet, or a list with mixed types. In Groovy, both can be used interchangeably.

The output of a pipeline step/mudules adheres to the same structure so that pipeline steps can easily be chained.

Step by step

Let us illustrate some key features of NextFlow together with how we use them in DiFlow and approach this step by step.

The code blocks below are run with the following version of NextFlow:

```
nextflow -v
nextflow version 20.10.0.5430
```

Step 1 - Operate on a stream

Let us illustrate the stream-like nature of a NXF channel using a very simple example: computing 1+1.

This chunk is directly taken from main.nf, running it can be done as follows:

```
nextflow run . -entry step1

N E X T F L O W ~ version 20.10.0

Launching `./main.nf` [backstabbing_cantor] - revision: d36e191fd1

WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
2
```

Step 2 - Operate on a stream in parallel

NextFlow (and streams in general) are supposed to be a good fit for parallel execution. Let's see how this can be done:

Running it can be done using:

```
nextflow run . -entry step2

N E X T F L O W ~ version 20.10.0

Launching `./main.nf` [furious_wing] - revision: d36e191fd1

WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE

2

3
4
```

Step 3 - Operate on a stream using a process

In the previous example, we ran 3 parallel executions each time applying the same simple function: adding one. Let us simulate now a more real-life example where parallel executions will not take the same amount of time. We do this by defining a process and workflow that uses this process. The rest is similar to our example before.

Running it is again the same.

```
nextflow run . -entry step3

N E X T F L O W ~ version 20.10.0

Launching `./main.nf` [zen_spence] - revision: d36e191fd1

WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE executor > local (3)

[5f/3dd3d9] process > step3:add (1) [ 33%] 1 of 3

2

executor > local (3)

[28/32e11f] process > step3:add (3) [100%] 3 of 3 

2

3

4
```

The result will be a permutation of 2,3 and 4. Try it multiple times to verify for yourself that the order is not guaranteed to be the same. Even though the execution times will not be that much different! In other words, a Channel does not guarantee the order, and that's a good thing.

Step 4 - How a map is not asynchronous

An illustrative test is one where we do not use a process for the execution, but rather just map but such that one of the inputs *takes longer* to process, i.e.:

Running it:

```
nextflow run . -entry step4

N E X T F L O W ~ version 20.10.0

Launching `./main.nf` [voluminous_montalcini] - revision: d36e191fd1

WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
2
3
4
```

The result may be somewhat unexpected, the order is retained even though there's a 2 second delay between the first entry and the rest. The sleep in other words blocks all the parallel execution branches.

This is a clear indication of why it's better to use a process to execute computations. On the other hand, as long as we *stay* inside the $_{map}$ and don't run a process, the order is retained. This opens up possibilities that we will exploit in what follows.

Step 5

If we can not guarantee the order of the different parallel branches, we should introduce a *branch ID*. This may be a label, a sample ID, a batch ID, etc. It's the unit of parallelization.

We can ran this code sample in the same way as the previous examples.

Please note that the function to add 1 remains exactly the same, we only added the id as the first element of the tuple in both input and output. As such we keep a handle on which sample is which, by means of the *key* in the tuple.

Note: Later, we will extend this tuple and add configuration parameters to it... but this was supposed to go step by step.

Step 6

What if we want to be able to configure the term in the sum? This would require a parameter to be sent with the process invocation. Let's see how this can be done.

This works, but is not very flexible. What if we want to configure the operator as well? What if we want to have branch-specific configuration? We can add a whole list of parameters, but that means that the process signature may be different for every process that we define. That is not a preferred solution.

Step 7

Let us use a simple hash to add 2 configuration parameters.

Step 8

Step 7 offers us a way to use a consistent API for a process. Ideally, however, we would like different process invocation to be chained rather than to explicitly add the correct configuration all the time. Let us add an additional key to the map, so that a process knows *it's scope*.

```
process addTupleWithProcessHash {
   input:
        tuple val(id), val(input), val(config)
   output:
        tuple val("${id}"), val(output)
   exec:
        def thisConf = config.addTupleWithProcessHash
        output = (thisConf.operator == "+") ? input + thisConf.term : input - thisConf.term
}

workflow step8 {
   Channel.from([1, 2, 3]) \
        | map{ el -> [ el.toString(), el, [ "addTupleWithProcessHash" : [ "operator" : "-", "term" : 10 ] ] ] } \
        | addTupleWithProcessHash \
        | view{ it }
```

Please note that we used the process name as a key in the map, so that each process can tell what configuration parameter are relevant for its own scope.

Step 9

We used native Groovy code in the process examples above. Let us now use a shell script:

```
workflow step8 {
    Channel.from( [ 1, 2, 3 ] ) \
        | map{ el -> [ el.toString(), el, [ "addTupleWithProcessHash" : [ "operator" : "-", "term" : 10 ] ] ] } \
        | addTupleWithProcessHash \
        | view{ it }
}
process addTupleWithProcessHashScript {
    input:
        tuple val(id), val(input), val(config)
    output:
        tuple val("${id}"), stdout
    script:
        def thisConf = config.addTupleWithProcessHashScript
        def operator = thisConf.operator
        def term = thisConf.term
        echo \$( expr $input $operator ${thisConf.term} )
```

Running this (in the same way as before), we get something along these lines:

```
[3, -7]
[1, -9]
[2, -8]
```

This is because the stdout qualifier captures the newline at the end of the code block. We could look for ways to circumvent that, but that is not the point here.

What's important to notice here:

- 1. We can not just retrieve individual entries in config in the shell, we have to let Groovy do that.
- 2. That means we either first retrieve individual values and store them in a variable,
- 3. or we use the $\{...\}$ notation for that.
- 4. If we want to use bash variables, the \$ symbol has to be escaped.

Obviously, passing config like this requires a lot of typing (especially as additional parameters are introduced) and is error prone.

Step 10

We used the pipe | symbol to combine different steps in a *pipeline* and we noticed that a process can do computations on parallel branches. That's nice, but we have not yet given an example of running 2 processes, one

after the other.

There are a few things we have to note before we go to an example:

- 1. It's not possible to call the same process twice, a strange error occurs in that case¹⁷.
- 2. If we want to pipe the output of one process as input of the next, the I/O signature needs to be exactly the same, so the output of the process should be a triplet as well.

¹⁷ It *is* possible in some cases however to manipulate the Channel such that a process is effectively run twice on the same data, but that is a more advanced topic.

```
process process_step10a {
    input:
        tuple val(id), val(input), val(term)
    output:
        tuple val("${id}"), val(output), val("${term}")
    exec:
        output = input.toInteger() + term.toInteger()
}
process process_step10b {
    input:
        tuple val(id), val(input), val(term)
        tuple val("${id}"), val(output), val("${term}")
    exec:
        output = input.toInteger() - term.toInteger()
}
workflow step10 {
    Channel.from( [ 1, 2, 3 ] ) \
        | map{ el -> [ el.toString(), el, 10 ] } \
        | process_step10a \
        | process_step10b \
        | view{ it }
}
```

The result of this is that first 10 is added and then the same 10 is subtracted again, which results in the same as the original. Please note that the output contains 3 elements, also the term passed to the process:

```
[3, 3, 10]
[1, 1, 10]
[2, 2, 10]
```

We can configure the second process (subtraction) by adding an additional map in the mix:

Please note that we define the closure in a different manner here, using the special variable it. We could also write (to the same effect):

```
...
| map{ x -> [ x[0], x[1], 5 ] } \
...
```

or even

```
...
| map{ id, value, term -> [ id, value, 5 ] } \
...
```

Step 11

What if we rewrite the previous using some of the techniques introduced earlier. Let us specify the operator as a parameter and try to stick to just 1 process definition.

```
process process_step11 {
    input:
        tuple val(id), val(input), val(config)
    output:
        tuple val("${id}"), val(output), val("${config}")
    exec:
        if (config.operator == "+")
           output = input.toInteger() + config.term.toInteger()
           output = input.toInteger() - config.term.toInteger()
}
workflow step11 {
    Channel.from([1, 2, 3]) \
        | map{ el -> [ el.toString(), el, [ "term" : 10, "operator" : "+" ] ] } \
        | process_step11 \
        | map{ id, value, term -> [ el.toString(), el, [ "term" : 11, "operator" : "-" ] ] } \
        | process_step11 \
        | view{ it }
}
```

This little workflow definition results in an error, just like we warned before:

There is, however, one simple way around this: include ... as ... Let us see how this works.

First, we store the process in a file examples/step/step11.nf:

```
input:
    tuple val(id), val(input), val(config)
output:
    tuple val("${id}"), val(output), val("${config}")
exec:
    if (config.operator == "+")
        output = input.toInteger() + config.term.toInteger()
    else
        output = input.toInteger() - config.term.toInteger()
```

The workflow definition becomes:

Running this yields an output similar to this:

```
$ nextflow run . -entry step11
N E X T F L O W ~ version 19.10.0
Launching `./main.nf` [sharp_gilbert] - revision: ee0b54f3d9
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (6)
[e3/aabcbc] process > step11:process_step11a (3) [100%] 3 of 3
[3e/ec7d8f] process > step11:process_step11b (3) [100%] 3 of 3
[2, -4]
[1, -5]
[3, -3]
```

We made a few minor changes to the workflow code in the meanwhile:

- 1. Splitting the conversion from an array of items to the triplet is now done explicitly and separate from the specifying the configuration for the process itself.
- 2. The view now only contains the relevant parts, not the configuration part for the last process.

The above example illustrates the include functionality of NextFlow DSL2. This was not possible with prior versions.

Step 12

Let's implement a simple map/reduce schema with what we developed above. Until now, we basically covered the mapping stage: starting from 3 independent number, execute a function on each *branch* individually. Now, we want to calculate the sum at the end (reduce phase).

We do this by adding a process to the example in Step 10

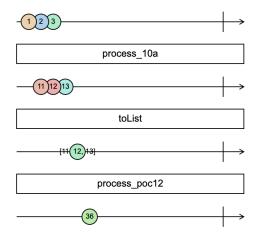
```
process process_step12 {
    input:
        tuple val(id), val(input), val(term)
    output:
        tuple val("${id}"), val(output), val("${term}")
    exec:
        output = input.sum()
}

workflow step12 {
    Channel.from([ 1, 2, 3 ] ) \
        | map{ el -> [ el.toString(), el, 10 ] } \
        | process_step10a \
        | tolist \
        | map{ [ "sum", it.collect{ id, value, config -> value }, [ : ] ] } \
        | view{ [ it[0], it[1] ] }
}
```

A few remarks are in order here:

- 1. We use the tolist operator on the output of process_step10a. This can be regarded as merging the 3 parallel branches into one branch. The result has the signature Channel[List[Triplet]]. This tolist operator only *outputs* something on the output Channel when all incoming branches have finished and the *merge* can effectively be performed.
- 2. It's important to note that what is passed through the pipe is still a channel, only the number of *branches*, *nodes*, or whatever you want to call it differs.
- 3. The long <code>map{["sum", ...}</code> line may seem complex at first, but it's really not. We take in <code>List[Triplet]</code> and convert this to <code>Triplet</code>. The first element of the triplet is just an identifier (<code>sum</code>). The last is the configuration map, but we don't need configuration for the sum. As the second element we want to obtain <code>List[Int]</code>, where the values are the 2nd element from the original triplets. The Groovy function <code>collect</code> on an array is like <code>map</code> in many other languages.

The marble diagram can be depicted conceptually as follows, where we note that in effect it's triplets rather than numbers that are contained in the marbles:



Please note that though we define the *pipeline* sequentially, the 3 numbers are first handled in parallel and only combined when calling tolist. Stated differently, parallelism comes for free when defining workflows like this.

Step 13

Let us tackle a different angle now and start to deal with files as input and output. In order to do this, we will mimic the functionality from earlier and modify it such that a file is used as input and output is also written to a file.

The following combination of process and workflow definition does exactly the same as before, but now from one or more files containing just a single integer number:

```
process process_step13 {
    input:
        tuple val(id), file(input), val(config)
    output:
        tuple val("${id}"), file("output.txt"), val("${config}")
    script:
        0.00
        a=`cat $input`
        let result="\$a + ${config.term}"
        echo "\$result" > output.txt
        .....
}
workflow step13 {
    Channel.fromPath( params.input ) \
        | map{ el -> [ el.baseName.toString(), el, [ "operator" : "-", "term" : 10 ] ]} \
        | process_step13 \
        | view{ [ it[0], it[1] ] }
```

While doing this, we also introduced a way to specify parameters via a con-

figuration file (nextflow.config) or from the CLI. In this case params.input points to an argument we should provide on the CLI, for instance:

```
$ nextflow run . -entry step13 --input data/input1.txt
N E X T F L O W ~ version 19.10.0
Launching `./main.nf` [gigantic_noether] - revision: 94d747c151
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (1)
[b1/57daf8] process > step13:process_step13 (1) [100%] 1 of 1
[input1, <...>/diflow/work/b1/57daf8f6a8ce6c1bc78f91c37cb466/output.txt]
```

Let's dissect a bit what is going one here...

- 1. We provide the input file data/input1.txt as input which gets automatically added to the params map as params.input.
- 2. The content of input1.txt is used in the simple sum just as before.
- 3. The output Channel contains the known triplet but this time the second entry is not a value, but rather a filename.

Please note that the file is output.txt is automatically stored in the unique work directory. We can take a look inside to verify that the calculation succeeded:

```
$ cat work/b1/57daf8f6a8ce6c1bc78f91c37cb466/output.txt
11
```

It seems the calculation went well, although one might be surprised by two things:

- 1. The output of the calculation is stored in some randomly generated work directory whereas we might want it somewhere more *findable*.
- 2. The process itself defines the value of the output filename, which may seem odd... and it is.

Taking our example a bit further and exploiting the fact that parallelism is natively supported by NextFlow as we've seen before, we can pass multiple input files to the same workflow defined above.

```
$ nextflow run . -entry step13 --input "$PWD/data/input*.txt"

N E X T F L O W ~ version 19.10.0

Launching `./main.nf` [peaceful_spence] - revision: 94d747c151

WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (3)
[1c/a214c2] process > step13:process_step13 (1) [100%] 3 of 3
[input2, <...>/diflow/work/a6/7dee09b191837e67afa1139b20d525/output.txt]
[input3, <...>/diflow/work/97/5261eeb055375d0779b1ee2645502c/output.txt]
[input1, <...>/diflow/work/1c/a214c221285fc4b4e9ad65cc5c5b98/output.txt]
```

Please note that we

- 1. provide the absolute path to the file
- 2. use a wildcard * to select multiple files
- 3. enclose the path (with wildcard) in double quotes to avoid shell globbing.

In the latter case, we end up with 3 output files, each named output.txt in their own respective (unique) work directory.

Step 14

Let us tackle one of the pain points of the previous example: output files are hidden in the work directory. One might be tempted to specify an output file in the process definition as such file("<somepath>/output.txt") but when you try this, it will quickly turn out that this does not work in the long run (though it may work for some limited cases).

NextFlow provides a better way to achieve the required functionality: $publishDir^{18}$. Let us illustrate its use with an example again and just adding the publishDir directive:

¹⁸ https://www.nextflow.io/do cs/latest/process.html?highlight =publish#publishdir

```
process process_step14 {
    publishDir "output/"
    input:
        tuple val(id), file(input), val(config)
        tuple val("${id}"), file("output.txt"), val("${config}")
    script:
        a=`cat $input`
        let result="\$a + ${config.term}"
        echo "\$result" > output.txt
        0.00
}
workflow step14 {
    Channel.fromPath( params.input ) \
        | map{ el -> [ el.baseName.toString(), el, [ "operator" : "-", "term" : 10 ] ]} \
        | process_step14 \
        | view{ [ it[0], it[1] ] }
```

This single addition yields:

```
$ nextflow run . -entry step14 --input data/input1.txt
N E X T F L O W ~ version 19.10.0
Launching `./main.nf` [tiny_jones] - revision: 630950ba4c
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (1)
[2b/be1b41] process > step14:process_step14 (1) [100%] 1 of 1
[input1, <...>/diflow/work/2b/be1b41b70db8a855bfb8f17a300796/output.txt]
$ cat output/output.txt
11
```

This example shows us a powerful approach to publishing data during our at the end of a pipeline. There is a similar drawback as for the output filenames, however, and that is that the process defines the output directory explicitly. But there is a different problem as well which can be observed when running on multiple input files:

```
$ nextflow run . -entry step14 --input "$PWD/data/input*.txt"
N E X T F L O W ~ version 19.10.0
Launching `./main.nf` [exotic_thompson] - revision: 630950ba4c
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (3)
[3b/007268] process > step14:process_step14 (1) [100%] 3 of 3
[input3, <...>/diflow/work/82/7ec0f8d6106b1d4d61a2cb64797e74/output.txt]
[input2, <...>/diflow/work/53/e25634a6bdd1613837a07cc7234617/output.txt]
[input1, <...>/diflow/work/3b/0072687d416807b80cdca62aa7ab41/output.txt]
$ cat output/output.txt
11
```

What do you think happens here? Yes, sure, we *publish* the same output.txt file three times and each time overwriting the same file. The last one is the one that persists.

Step 15

Let us describe a way to avoid the above issue. There are other approaches to resolve this issue, but let us for the moment look at one that can easily be reused.

```
process process_step15 {
    publishdir "output/${config.id}"
    input:
        tuple val(id), file(input), val(config)
    output:
        tuple val("${id}"), file("output.txt"), val("${config}")
    script:
        0.00
        a=`cat $input`
        let result="\$a + ${config.term}"
        echo "\$result" > output.txt
        0.00
}
workflow step15 {
    channel.frompath( params.input ) \
        | map{ el -> [ el.basename.tostring(), el, [ "id": el.basename, "operator" : "-", "term" : 10 ] ]} \
        | process_step15 \
        | view{ [ it[0], it[1] ] }
```

This results in the following:

```
$ nextflow run . -entry step15 --input "$PWD/data/input*.txt"
N E X T F L O W ~ version 19.10.0
Launching `./main.nf` [berserk_gutenberg] - revision: 474b7b0a5b
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (3)
[5f/15f0a5] process > step15:process_step15 (3) [100%] 3 of 3
[input2, <...>/diflow/work/eb/30b10c68b03542373b340e08b2fb88/output.txt]
[input1, <...>/diflow/work/d6/cdd3aa7leab634c017f0eb6e44713c/output.txt]
[input3, <...>/diflow/work/5f/15f0a5ed44810731197fcb5f9893e7/output.txt]

$ cat output/input*/output.txt

11
12
13
```

In other words, since (in this case 3) parallel branches each write to the same output location we have to make sure that we add something unique for every of the parallel branches. Another approach is to tweak the name of the output file in the process, but for the moment it is still fixed and defined in the process itself. Let us take a look at that aspect next.

Step 16

We want the output filename to be configurable. That means that we either use the params map for this (and take care it is available in modules that are included) or we pass it to the process as part of the input. Let us explore both scenarios.

But first, we need to understand a bit better where the contents of params comes from. We already covered a few examples where we specify a params key on the CLI. There is another way as well, via nextflow.config. In it, we can add a scope params and add configuration there.

Let us reconsider the previous example (step15) but this time add a nextflow.config file like this (please update the <...> part according to your situation):

```
params.input = "<...>/diflow/data/*.txt"
```

Let us illustrate the effect by means of two examples:

```
> nextflow run . -entry step15
N E X T F L O W \sim version 19.10.0
Launching `./main.nf` [elated_poincare] - revision: 474b7b0a5b
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (3)
[45/12e2ed] process > step15:process_step15 (1) [100%] 3 of 3
[input2, <...>/diflow/work/62/102c68dde4382be33f028affec2245/output.txt]
[input3, <...>/diflow/work/f9/b6beedb0d82c3a8b9068bf02d41a2f/output.txt]
[input1, <...>/diflow/work/45/12e2ed9f6eb96905d1c213c00a8ea2/output.txt]
> nextflow run . -entry step15 --input data/input1.txt
N E X T F L O W ~ version 19.10.0
Launching `./main.nf` [pedantic_ritchie] - revision: 474b7b0a5b
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (1)
[b7/4462c7] process > step15:process_step15 (1) [100%] 1 of 1
[input1, <...>/diflow/work/b7/4462c7dcd558c5c1824eb1831d3ca5/output.txt]
```

In other words, params can be defined in nextflow.config but if it appears on the CLI then the latter gets priority. Please be reminded that params is a map, the following is equivalent:

```
params {
    input = "<...>/diflow/data/*.txt"
}
```

Step 16 - Add the output file to params

In this case, we would add a output = ... key to nextflow.config or provide --output ... on the CLI. This is done in the following example:

```
process process_step16 {
    publishDir "output/${config.id}"
    input:
        tuple val(id), file(input), val(config)
        tuple val("${id}"), file(params.output), val("${config}")
    script:
        a=`cat $input`
        let result="\$a + ${config.term}"
        echo "\$result" > ${params.output}
        0.00
}
workflow step16 {
    Channel.fromPath( params.input ) \
        | map{ el -> [ el.baseName.toString(), el, [ "id": el.baseName, "operator" : "-", "term" : 10 ] ]} \
        | process_step16 \
        | view{ [ it[0], it[1] ] }
```

The result is

```
> nextflow run . -entry step16 --input data/input1.txt --output output1.txt
N E X T F L O W ~ version 19.10.0
Launching `./main.nf` [drunk_jang] - revision: e6935c0bab
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE executor > local (1)
[61/158709] process > step16:process_step16 (1) [100%] 1 of 1
[input1, <...>/diflow/work/61/1587094bd416db4d108b2bd0aff340/output1.txt]
> cat output/input1/output1.txt
```

We note that the params.output occurs in the output: triplet as well as in the script code itself. That's quite important, otherwise NextFlow will complain the output file can not be found.

This approach does what it is supposed to do: make the output filename configurable. There are a few drawbacks however:

- 1. We would have to configure the filename for *every* process individually. While this can be done (params.cprocess>.output for instance), it requires additional bookkeeping on the side of the pipeline developer.
- 2. It does not help much because the output filename for every parallel branch again has the same name. In other words, we still have to have the publishbir

In all fairness, these issues only arise when you want to *publish* the output

data because in the other case every process lives in its own work directory.

Step 17 - Add the output filename to the triplet

The other approach to take is to add the output filename to the triplet provided as input to the process. This can be done similarly to what we did with the input filename, i.e.:

```
process process_step17 {
    publishDir "output"
    input:
        tuple val(id), file(input), val(config)
    output:
        tuple val("${id}"), file("${config.output}"), val("${config}")
        0.00
        a=`cat $input`
        let result="\$a + ${config.term}"
        echo "\$result" > ${config.output}
}
workflow step17 {
    Channel.fromPath( params.input ) \
        | map{ el -> [
            el.baseName.toString(),
            el,
            [
                "output" : "output_from_${el.baseName}.txt",
                "id": el.baseName,
                "operator" : "-",
                "term" : 10
            ]
          ]} \
        | process_step17 \
        | view{ [ it[0], it[1] ] }
}
```

In order to make a bit more sense of the (gradually growing) configuration map that is sent to the process, we tuned the layout a bit. In this case, the output filename that is configured contains an identifier for the input as well. In this way, the output is always unique.

Since we have configured params.input in nextflow.config, we are able to just run our new *pipeline*:

```
$ nextflow run . -entry step17
N E X T F L O W ~ version 19.10.0
Launching `./main.nf` [modest_kilby] - revision: 8c97318d5a
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (3)
[30/9658c3] process > step17:process_step17 (1) [100%] 3 of 3
[input3, <...>/diflow/work/bb/a820f42cc1f099d9308f14c11da797/output_from_input3.txt]
[input2, <...>/diflow/work/81/32f59c31bc0a355828397994f5a5d0/output_from_input2.txt]
[input1, <...>/diflow/work/30/9658c3eb08ceabc6f0fb3e07449dec/output_from_input1.txt]

$ ls -1 output/
output_from_input2.txt
output_from_input3.txt
```

In other words, this allows to distinguish between parallel branches in the pipeline.

Please note that if we add steps to the *pipeline*, because the output is reported as input for the next process, it automatically points to the correct filename even though the next process is not aware of the way the output filename has been specified. That's nice.

Step 18 - Use a closure

We mentioned that there are 2 ways to pass an output filename to a process. There is a third one, using a closure or function to handle the naming for us.

Let us illustrate this with an example again:

```
def out_from_in = { it -> it.baseName + "-out.txt" }
process process_step18 {
    publishDir "output"
    input:
        tuple val(id), file(input), val(config)
    output:
        tuple val("${id}"), file("${out}"), val("${config}")
    script:
        out = out_from_in(input)
        0.00
        a=`cat $input`
        let result="\$a + ${config.term}"
        echo "\$result" > ${out}
        0.00
}
workflow step18 {
    Channel.fromPath( params.input ) \
        | map{ el -> [
            el.baseName.toString(),
            el,
            Ε
                "id": el.baseName,
                "operator" : "-",
                "term" : 10
            ]
          ]} \
        | process_step18 \
        | view{ [ it[0], it[1] ] }
}
```

The result is as follows:

```
$ nextflow run . -entry step18
N E X T F L O W ~ version 19.10.0
Launching `./main.nf` [gigantic_shockley] - revision: 696b9c6ef1
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (3)
[e6/3f62e5] process > step18:process_step18 (1) [100%] 3 of 3
[input2, <...>/diflow/work/d4/8c78167d730ebe7e8150e899d792c8/input2-out.txt]
[input3, <...>/diflow/work/c0/20bbad0e0ca811634aed8673a63726/input3-out.txt]
[input1, <...>/diflow/work/e6/3f62e5749072fa636836da95574f3c/input1-out.txt]
```

We can even add the closure to the configuration map sent to the process, but NextFlow complains that this is not serializable so you may miss some features and most importantly it may not work at all times:

WARN: Cannot serialize context map. Cause: java.lang.IllegalArgumentException: Unknown workflow parameter definit – Resume will not work on this process

This approach may seem like completely over-engineered but for a lot of use-cases it turns out to be a good fit. Although, not in the way we introduced it here. We come back to that later...

Step 20

We touch upon a point that we have encountered but not really considered in-depth: the order of *things* in the channel or stream. We've noticed that the order is not predictable and we've discussed that this is to be expected. In general, the duration of a process step may depend on the data or the number of resources available at the time of running. Also, the example where we joined the different parallel branches (Step 12 - **REF**) was independent of the order because it just calculated the sum.

Another consequence of the undetermined order of *events* is the fact that during a join or reduce phase (for instance with toList), the resulting order is undetermined and this messes up the caching functionality of NextFlow.

Let us give an example with a reduce process that *does* depend on the order of *events*. We divide the first element from the *map* phase by the second one:

If you run this code like this, you get something like this when launching multiple times:

```
$ nextflow run . -entry step20 -with-docker
N E X T F L O W ~ version 19.10.0
Launching `./main.nf` [awesome_bernard] - revision: f2b9ccb088
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (3)
[e4/7ca36c] process > step20:process_step10a (2) [100%] 2 of 2
[03/2027f4] process > step20:process_step20
                                               [100%] 1 of 1
[sum, 0.9166666667]
$ nextflow run . -entry step20 -with-docker
N E X T F L O W \sim version 19.10.0
Launching `./main.nf` [hopeful_majorana] - revision: f2b9ccb088
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
executor > local (3)
[ad/8ad0ca] process > step20:process_step10a (1) [100%] 2 of 2
[85/9fb964] process > step20:process_step20
                                                 [100%] 1 of 1
[sum, 1.0909090909]
```

Luckily, there is a variant of the tolist channel operator that takes into account sorting: toSortedList. There are other operators as well, but we leave it as an exercise to look those up. The workflow code above simply becomes:

In this example, we sort (alphabetically) on the id in the triplet.

Step A1

Let us consider a different example: running a CLI tool inside the script block that takes arguments. We will assume (at least for now) that the tool is in the \$PATH of the execution environment. Since we are not (yet) running inside a container, we make the switch to Docker first.

Extras

Step A2 - Conditional logic

Let us consider a different topic: high-level pipeline logic. Sometimes, one want to provide the option to run just part of a pipeline, or support branches in the logic depending on a parameter or even a result of a pipeline processing step.

Let us assume a couple of steps in a pipeline, each represented by a $_{\sf map}$ to make the code easier to read. The code below splits apart the logic of running a specific step from the one of the pipeline itself.

```
workflow runOrSkip {
    take:
    data_
                 // Data Channel
    thisProcess // The map, process or workflow to run
               // Function/closure to check if step needs to run, returns Boolean
    runOrNot
    thisStep
                  // The current step to run or not
    main:
    runStep_ = data_.branch{ it ->
           run: runOrNot(thisStep)
            skip: ! runOrNot(thisStep)
       }
    step_ = runStep_.run \
        | thisProcess \
        | mix(runStep_.skip) \
    emit:
    step_
}
def runOrNot(thisStep) {
   def STEPS = [ "step1", "step2", "step3", "step4", "step5" ]
   def steps = params.steps.split(",")
                    .collect{ it ->
                        (it.contains("-"))
                            ? STEPS[STEPS.indexOf(it.split("-")[0])..STEPS.indexOf(it.split("-")[1])]
                            : it
                    }.flatten()
    return steps.contains(thisStep)
}
workflow stepA2 {
    input_ = Channel.from( [ 1, 2, 3 ] )
    step1_ = runOrSkip(input_, map{ it -> it * 2 }, runOrNot, "step1")
    step2_ = runOrSkip(step1_, map{ it -> it + 5 }, runOrNot, "step2")
    step3_ = run0rSkip(step2_, map{ it -> it / 2 }, run0rNot, "step3")
    step4_ = run0rSkip(step3_, map{ it -> it + 1 }, run0rNot, "step4")
    step5_ = runOrSkip(step4_, map{ it -> it + 5 }, runOrNot, "step5")
    step5_.view{ it }
```

The result is exactly what we wanted, a flexible approach to selecting possible steps in a pipeline:

```
$ NXF_VER=20.04.1-edge nextflow run . -entry stepA2 -with-docker --steps "step1-step3,step5"
N E X T F L O W ~ version 20.04.1-edge
Launching `./main.nf` [drunk_becquerel] - revision: 3672a5b1b7
WARN: DSL 2 IS AN EXPERIMENTAL FEATURE UNDER DEVELOPMENT -- SYNTAX MAY CHANGE IN FUTURE RELEASE
8.5
9.5
10.5
```

Please note that we do perform any checks on whether the steps parameter is provided or it has the correct format. We leave this as an exercise.

Variables in nextflow.config

CLI arguments and options for specific components/steps in the pipeline are configured in the respective <code>nextflow.config</code> files that are imported in the global one. But that also means that we can not override them from the CLI anymore. For instance, it is not possible to add an argument in the style <code>--component.input.value <value></code>. That means that all options would either be fixed for the whole pipeline, or to be configured in <code>nextflow.config</code> explicitly. The latter is possible by means of a custom config file that overrides the other settings.

There is, however, an easier approach to this: variables in <code>nextflow.config</code>. The functionality is explained here¹⁹ and is used in DiFlow for allowing us to provide the (scoped) parameter values on the CLI. For instance, this is an excerpt from an existing component's <code>nextflow.config</code>:

¹⁹ https://www.nextflow.io/do cs/latest/config.html#configvariables

```
params {
    ...
    cellranger_vdj__id = "cr"
    ...
    cellranger_vdj {
        name = "cellranger_vdj"
        container = "mapping/cellranger_vdj/cellranger_vdj:4.0.0-1"
        command = "cellranger_vdj"
        arguments {
          ...
        id {
              name = "id"
              otype = "--"
              value = "${params.cellranger_vdj__id}"
          ...
        }
        ...
}
```

If you look at this one parameter for the cellranger_vdj component, you notice that directly under params, we have the key cellranger_vdj__id. In other words, the component name followed by a double underscore and then the parameter name. Since all arguments are named here, we do not have to have to specify -'s or --'s.

Appendix

Caveats and Tips

Resources

When you run or export with the <code>DockerTarget</code>, resources are automatically added to the running container and stored under <code>/resources</code>. In case of the <code>NativeTarget</code>, this is not the case and since <code>NextFlowTarget</code> uses the <code>NativeTarget</code> it's the same there. That does not mean that resources specified in <code>functionality.yaml</code> is not available in these cases, we only have to point to them where appropriate.

The following snippet (from ct/singler) illustrates this:

```
par = list(
  input = "input.h5ad",
  output = "output.h5ad",
  reference = "HPCA",
  outputField = "cellType",
  pruningMADS = 3,
  outputFieldPruned = "celltype-pruned",
  reportOutputPath = "report.md"
)
## VIASH END
par$resources_dir <- resources_dir</pre>
```

In other words, <code>resources_dir</code> is automatically created by <code>viash</code> in all current 3 environments. This means that we can point to the <code>report.Rmd</code> file present in the resources like so:

```
rmarkdown::render(paste0(par$resources_dir, "/", "report.Rmd"), output_file = par$reportOutputPath)
```

Default values

In functionality, no option should have an empty string as value!

```
target_image
```

It makes sense to add the target_image attribute in the docker_platform.yaml file. This way, the resulting container image is predictable, rather than an autogenerated tag from viash.

Running the Docker setup

We don't have a solution yet for pre-generating the Docker images prior to starting a NXF pipeline. For the moment, we ask the user to run the build script for the Docker targets with the ---setup option. This only works locally, it would for instance not work on a different (clean) node or in a Kubernetes cluster.

We are working on solutions or workarounds for this. Keep you posted!

Open issues

- 1. Multiple files as input for a component: E.g. the concat component uses multiple files to be joined. At the moment this does not seems to be possible.
- 2. Use of additional input files into a specific component. Some components do not only have input/output but require additional input. How should we map this?