How to Package an Algorithm with Algorun

A docker-based packaging system v1.1

ABSTRACT

AlgoRun is a dedicated packaging system for computational algorithms. This document shows how to package an algorithm with AlgoRun and an example of Bowtie software.

1 Introduction

AlgoRun is a docker-based software container template designed to package computational algorithms. This document shows steps of how to create an AlgoRun container of the Bowtie software.

2 Download Docker

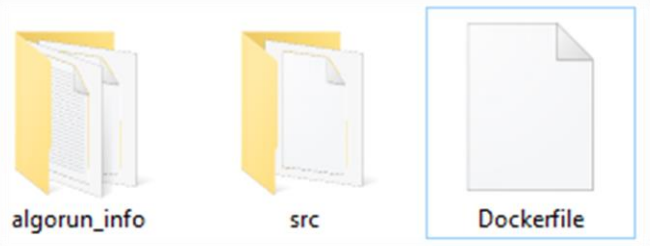
Before starting, download and install Docker on your local machine. Docker can be installed on Mac OS, Linux as well as Windows. Follow the instructions on: https://docs.docker.com/v1.8/installation/

3 Download AlgoRun

AlgoRun is a Docker container template to make packaging algorithms a straightforward process. Download AlgoRun from: http://algorun.org/resources/skeleton.zip

4 Steps to Create an AlgoRun container

Unzip the previously downloaded zip file. The resulting folder has the following structure:



- Docker builds a software container automatically by reading the instructions from Dockerfile. A Dockerfile is a text document that contains all commands needed to build the software container.
- AlgoRun template container uses the `src` and `algorun_info` folders to describe a computational algorithm in a standard format.

STEP 1:

Add all source code files of your algorithms into the `src` folder.

STEP 2:

Edit the `Dockerfile` to make sure your algorithm dependencies will get installed in the container. AlgoRun is based on Ubuntu 15.10 Linux system. So, you can leverage Ubuntu packaging system to get your dependencies installed.

> *Example:* `RUN apt-get install -y build-essential` *to install C++ compiler*

For more information about Dockerfile, please refer to the Docker documentation (https://docs.docker.com/v1.8/reference/builder/).

STEP 3:

Edit the `manifest.json` file inside the `algorun_info` folder. Below is an example of the manifest file.

```
{
  "algo_name": "SDDS",
  "algo_summary": "Stochastic Discrete Dynamical System",
  "algo_description": "SDDS module simulates the average trajectory for each variable out of numberofSimulations trajectories deterministically or stochastically",
  "algo_website": "http://algorun.org",
  "algo_keywords": ["reverse engineering", "cell biology"],
  "algo_authors": [
    {"name": "Seda Arat","email": "arat@uchc.edu","profile_picture": "","personal_website": "http://www.math.vt.edu/people/sedag/","organization": "Center for Quantitative Medicine","org_website": "http://cqm.uchc.edu/"
    }
  ],
  "algo_exec": "ruby Sdds.rb",
  "algo_input_stream": "file",
  "algo_output_stream": "output.txt",
  "algo_parameters": {
  },
  "input_type": "algorun:superadam",
  "algo_image": "algorun/sdds"
}
```

*Source code: an example of **manifest.json** file*

In addition to adding algorithm's information, the following fields are necessary for AlgoRun to correctly run the algorithm source code:

- "`algo_exec`": is the command used to start algorithm executed.
- "`algo_input_stream`": is how the algorithm reads the input data. Values can be one of the following:
  - `direct`: if the algorithm input is passed directly as the first parameter in the command line.
  - `file`: if the algorithm reads input from a file. File name is then passed as the first command line argument.
  - `stdin`: if the input is passed through the standard input stream using '<' operator.
- "`algo_output_stream`": is the path of the file where the algorithm outputs its result or `stdout` if the algorithm prints the result to the standard output stream.

Command line options can be exposed in the "`algo_parameters`" field[1]. AlgoRun website uses "`input_type`" field to easily categorize algorithms that can work together in a standard data format. Users can also download and use the algorithm Docker image locally from Docker Hub if the value "`algo_image`" is provided[2].

STEP 4:

Provide input and output examples in the `input_example.txt` and `output_example.txt` files respectively.

[1] More details about using parameters in section 7.
[2] More details about publishing algorithms to the AlgoRun website in section 9.

STEP 5:

Build the algorithm container using `docker build` command.

Example: `docker build -t <algorithm_name> .`

5 EXAMPLE: Packaging Bowtie Software with AlgoRun

Bowtie is an ultra-fast memory-efficient short read aligner[3]. The source code is written in C++ and is available under the Artistic License. Download it from http://sourceforge.net/projects/bowtie-bio/files/bowtie/1.1.2/

Unzip the downloaded file. It results in a folder containing all the source code of Bowtie.

STEP 1:

- Add all Bowtie source files inside the `src` folder.

STEP 2:

- Install C++ dependencies in Dockerfile. In addition, build the source code using `make` command. Below is how the Dockerfile of Bowtie looks like.

```
1  FROM algorun/algorun
2
3  ADD ./algorun_info /home/algorithm/web/algorun_info/
4  ADD ./src /home/algorithm/src/
5
6  # Install any algorithm dependencies here
7  RUN apt-get update && apt-get install -y build-essential
8  RUN cd /home/algorithm/src && make
```

Source code: Dockerfile of Bowtie software

Hints:

1. Dockerfile syntax requires to precede all commands with `RUN` keyword.
2. To ensure successful installation, always use apt-get update before installing packages and use -y option in the install command.
3. Change to `/home/algorithm/src` directory before running any command that operates on the source files inside `src` folder.

[3] For more information: visit Bowtie website: http://bowtie-bio.sourceforge.net/index.shtml

STEP 3:

- `manifest.json` file is required to describe the computational algorithm. Comments in the file will guide you to fill the correct values. Below is how the manifest of Bowtie looks like.

```
{
  "algo_name": "Bowtie 1.1.2",
  "algo_summary": "Bowtie is an ultrafast, memory-efficient alignment program for aligning short DNA sequence reads to large genomes.",
  "algo_description": "Bowtie is an ultrafast, memory-efficient short read aligner geared toward quickly aligning large sets of short DNA sequences (reads) to large genomes. Check <a href='http://bowtie-bio.sf.net/' target='_blank'>our website</a> for detailed explanation. This interface is meant to provide a quick and easy access to the computation without having to install Bowtie packages. Command line options are exposed as parameters, which you can configure from the above window.",
  "algo_website": "http://bowtie-bio.sf.net/",
  "algo_keywords": ["bowtie", "DNA", "genome", "sequencing", "alignment", "Burrows-Wheeler", "indexing"],
  "algo_authors": [
    {
      "name": "Ben Langmead",
      "email": "langmead@cs.umd.edu",
      "profile_picture": "ben.jpg",
      "personal_website": "http://www.cs.jhu.edu/~langmea/",
      "organization": "John Hopkins University",
      "org_website": "https://www.jhu.edu/"
    },
    {
      "name": "Cole Trapnell",
      "email": "coletrap@uw.edu",
      "profile_picture": "cole.png",
      "personal_website": "http://cole-trapnell-lab.github.io/team/cole-trapnell/",
      "organization": "University of Washington",
      "org_website": "http://www.uw.edu/"
    }
  ],
  "algo_exec": "./bowtie e_coli -c",
  "algo_input_stream": "direct",
  "algo_output_stream": "stdout",
  "algo_parameters": {},
  "input_type": "algorun:dna-sequence",
  "algo_image": "algorun/bowtie"
}
```

*Source Code: **manifest.json** of Bowtie software (comments-skimmed)*

STEP 4:

- `input_example.txt` file includes a sample input data for users to quickly try the algorithm. Enter `ATGCATCATGCGCCAT` as an example.
- `output_example.txt` file includes a sample of the expected output for the same input. It makes it easier for users to expect the results. The above input produces the following:

```
0     -     gi|110640213|ref|NC_008253.1| 148810      ATGGCGCATGATGCAT
      IIIIIIIIIIIIIIII  0     10:A>G,13:C>G
```

NOTES

- Bowtie source code comes with `e_coli` index packaged by default. So, use it the `algo_exec`. If you included other indexes, it's ok to use them as well.
- Use `direct` in `algo_input_stream` to accept input directly from the command line. Bowtie has other options to read the input from a file. However, AlgoRun will automatically present an option to upload a file to the input area in the web interface.
- Use `stdout` in `algo_output_stream` to let AlgoRun catch the result from the terminal. Bowtie has other options to write the output to a file. However, AlgoRun will automatically present an option to download the result to a file from the web interface.

STEP 5:

- From the directory where the Dockerfile exists, build Bowtie container using:
  `docker build -t bowtie .`
- You should see a success message as in the following picture.

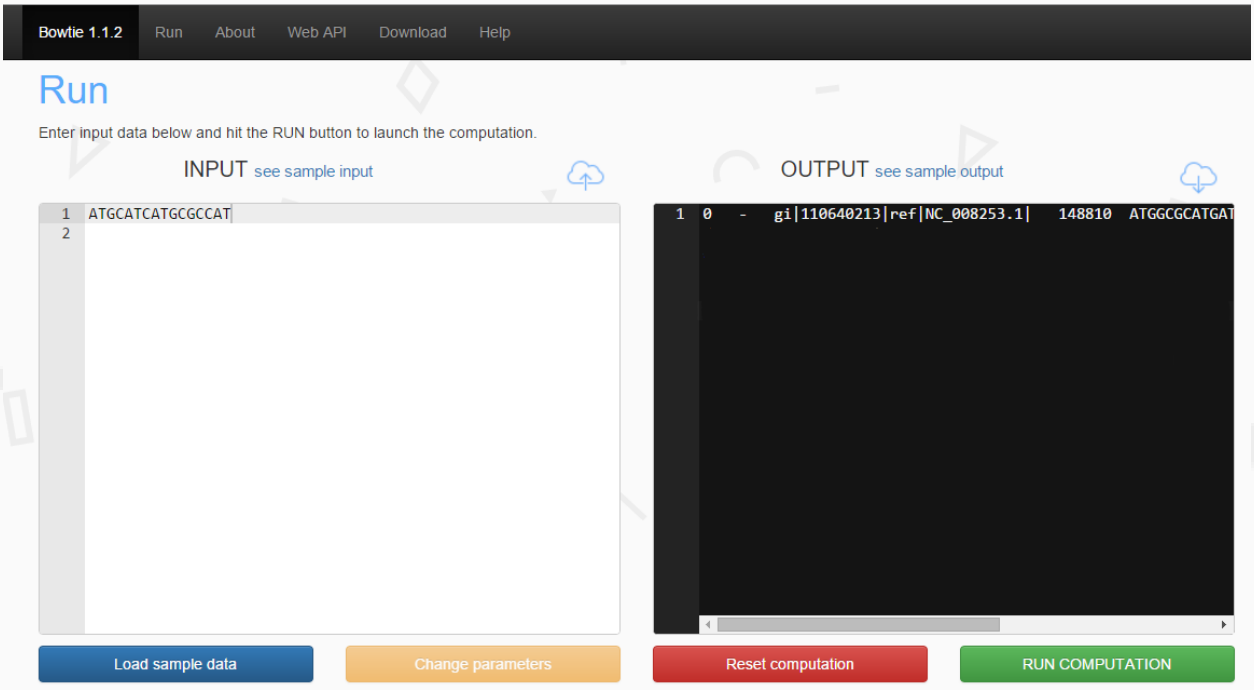
```
 ---> 0788ef071b7e
Removing intermediate container e6d52cdf612c
Step 6 : MAINTAINER Abdelrahman Hosny <abdelrahman.hosny@hotmail.com>
 ---> Running in 5c9d49c5c70f
 ---> 6e1bfa3d638f
Removing intermediate container 5c9d49c5c70f
Successfully built 6e1bfa3d638f
abdelrahman@abdelrahman-laptop:~/uchc/algorun/examples/bowtie-1.1.2$
```

Bowtie container build success message

6 User Interface

Run Bowtie container using:
`docker run -p 31331:8765 bowtie`

Open the web browser and type http://localhost:31331



Hint: You can use any available port other than 31331. Yet, you must bind it to 8765 port as it is the gateway to AlgoRun.

7 [OPTIONAL] Expose Command Lind Options as Parameters

To give a computational algorithm flexibility, AlgoRun allows to expose parameters that can be easily changed from the web interface. These parameters will be available as environment variables in the source code.

The power of Bowtie as a very fast DNA sequences aligner comes from the available command line options. So, you can make use of AlgoRun parameters to expose these command line options. You have two options: either to manipulate the source code of Bowtie so that it reads options from environment variables (instead of command line) or to develop a wrapper around Bowtie main executable that will internally translate environment variables to command line options. To do so, follow the below steps:

The example here uses Ruby programming language to write the wrapper. You can use any other language and apply the same concepts.

1. Specify parameters and their default values in the manifest file. The adjacent picture shows some parameters.
2. Read the input data[4]. The input data is passed as the first command line argument.
3. Read the environment variables (of the same names you specified in the manifest) and form the options string.
4. Call the executable file and to print the output to the standard output[5].

```
28  "algo_parameters": {
29    "Skip": "0",
30    "Only-Align": "all",
31    "Trim-Left": "0",
32    "Trim-Right": "0",
33    "Phred-Quality": "33",
34    "Solexa": "off",
35    "Align-v": "0",
36    "Align-n": "2",
37    "Align-e": "70",
38    "Align-l": "28",
39    "Align-I": "0",
40    "Align-X": "250",
41    "Report-k": "1",
42    "Report-all": "off",
43    "Report-m": "no-limit",
44    "Report-best": "off",
45    "Report-strata": "off",
46    "suppress": "0"
47  },
```

Modify the Dockerfile to install ruby dependency:

```
7  RUN apt-get update && apt-get install -y ruby build-essential
```

Modify `algo_exec` value in the manifest file to:

```
25    "algo_exec": "ruby bowtie.rb",
```

Rebuild Bowtie container using: `docker build -t bowtie .`

[4] Remember that you can use “direct”, “file” or “stdin” alternatives to read the input. Whatever you choose, modify the manifest file accordingly.

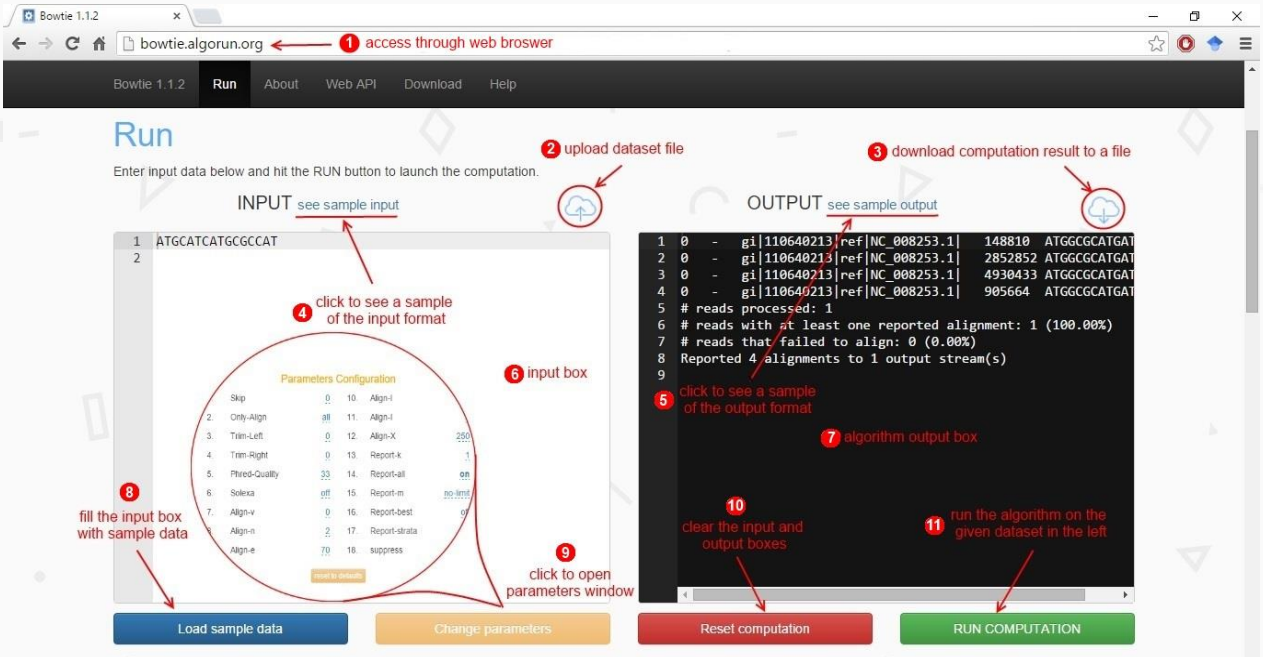
[5] You can also write the output to a file and specify the file name in the manifest key “algo_output_stream”

```ruby
require 'open3'

# read input data that is passed directly
input_data=ARGV[0].strip

# form the options string by reading envirnment variables
options = ""

options += " -s " + ENV["Skip"].strip
options += " -u " + ENV["Only-Align"].strip unless ENV["Only-Align"] == "all"
options += " -5 " + ENV["Trim-Left"].strip
options += " -3 " + ENV["Trim-Right"].strip
options += " --phred64-quals" if ENV["Phred-Quality"] == "64"
options += " --solexa-quals" if ENV["Solexa"] == "on"
options += " -n " + ENV["Align-n"].strip
options += " -v " + ENV["Align-v"].strip
options += " -n " + ENV["Align-n"].strip
options += " -e " + ENV["Align-e"].strip
options += " -l " + ENV["Align-l"].strip
options += " -I " + ENV["Align-I"].strip
options += " -X " + ENV["Align-X"].strip
options += " -k " + ENV["Report-k"].strip
options += " --all" if ENV["Report-all"] == "on"
options += " -m " + ENV["Report-m"].strip unless ENV["Report-m"] == "no-limit"
options += " --best" if ENV["Report-best"] == "on"
options += " --strata" if ENV["Report-strata"] == "on"
options += " --suppress " + ENV["suppress"].delete(' ') unless ENV["suppress"] == "0"
options.strip!

# run the algorithm with the options injected
command = "./bowtie " + options + " e_coli -c " + input_data
stdin, stdout, stderr, wait_thr = Open3.popen3(command)

# print the output to the standard output stream
puts stdout.read
puts stderr.read
```

*Source Code: **bowtie.rb** wrapper code*

At this point, options available from Bowtie can be changed by clicking on “Change Parameters” button from the web interface. Visit http://bowtie.algorun.org for the final version of Bowtie running inside AlgoRun standard container.

Find the complete example on AlgoRun GitHub repository (https://github.com/algorun/algorun).

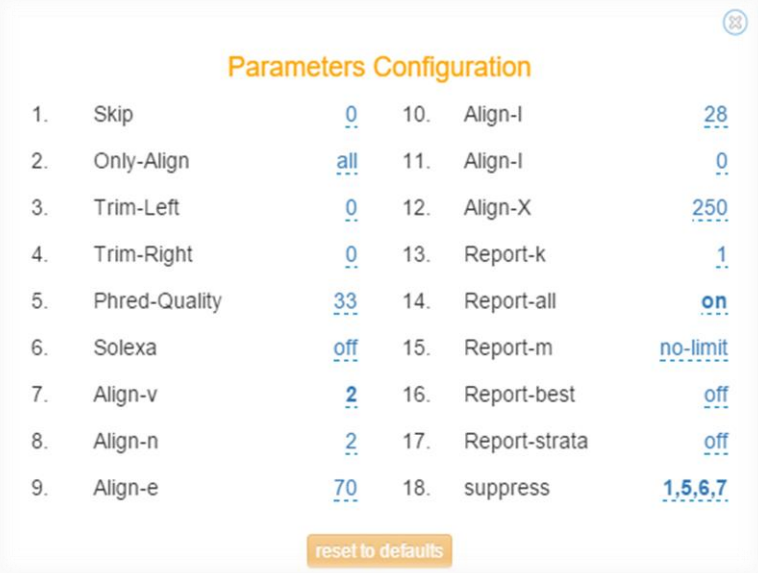


Bowtie web interface

8 Examples (Command Line Options vs. Parameters)

8.1.

Example Link: http://bowtie-bio.sourceforge.net/manual.shtml#example-1--a
Command line: `./bowtie -a -v 2 e_coli --suppress 1,5,6,7 -c ATGCATCATGCGCCAT`
With AlgoRun: Change `Report-all` to on, `Align-v` to 2 and `suppress` to 1,5,6,7



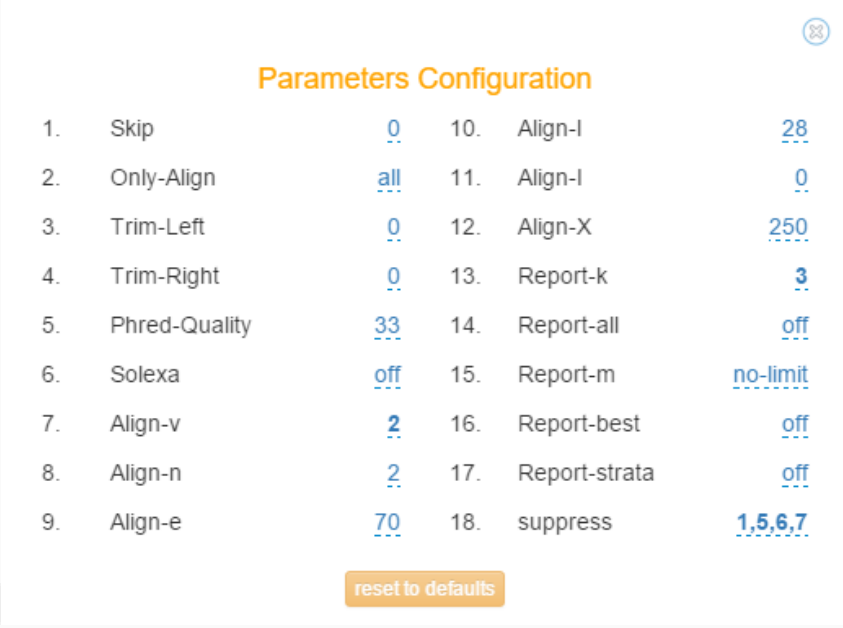
Parameters Configuration

1.	Skip	0	10.	Align-I	28
2.	Only-Align	all	11.	Align-I	0
3.	Trim-Left	0	12.	Align-X	250
4.	Trim-Right	0	13.	Report-k	1
5.	Phred-Quality	33	14.	Report-all	on
6.	Solexa	off	15.	Report-m	no-limit
7.	Align-v	2	16.	Report-best	off
8.	Align-n	2	17.	Report-strata	off
9.	Align-e	70	18.	suppress	1,5,6,7

reset to defaults

8.2.

Example Link: http://bowtie-bio.sourceforge.net/manual.shtml#example-2--k-3
Command line: `./bowtie -k 3 -v 2 e_coli --suppress 1,5,6,7 -c ATGCATCATGCGCCAT`
With AlgoRun: Change `Report-k` to 3, `Align-v` to 2 and `suppress` to 1,5,6,7



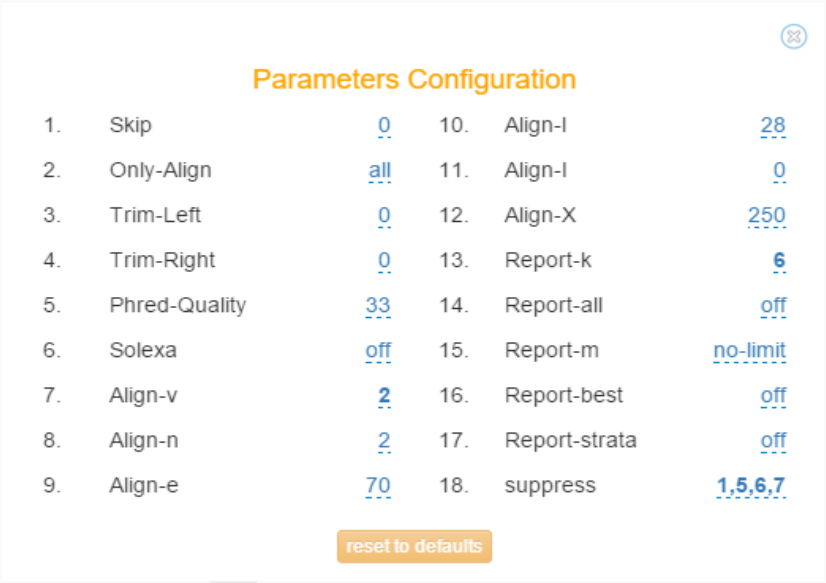
Parameters Configuration

1.	Skip	0	10.	Align-I	28
2.	Only-Align	all	11.	Align-I	0
3.	Trim-Left	0	12.	Align-X	250
4.	Trim-Right	0	13.	Report-k	3
5.	Phred-Quality	33	14.	Report-all	off
6.	Solexa	off	15.	Report-m	no-limit
7.	Align-v	2	16.	Report-best	off
8.	Align-n	2	17.	Report-strata	off
9.	Align-e	70	18.	suppress	1,5,6,7

reset to defaults

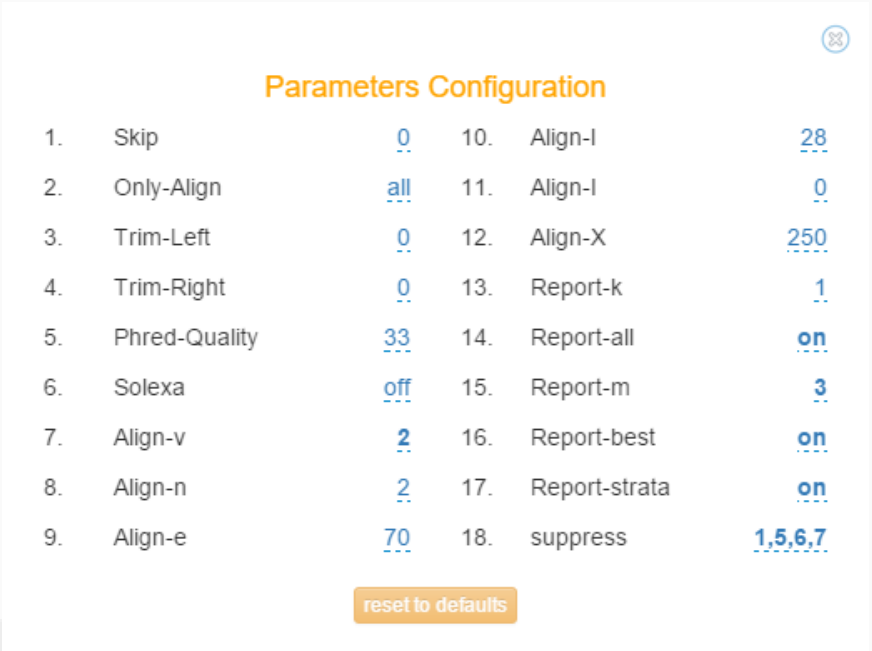
8.3.

Example Link: http://bowtie-bio.sourceforge.net/manual.shtml#example-3--k-6
Command line: `./bowtie -k 6 -v 2 e_coli --suppress 1,5,6,7 -c ATGCATCATGCGCCAT`
With AlgoRun: Change `Report-k` to 6, `Align-v` to 2 and `suppress` to 1,5,6,7



8.4.

Example Link: http://bowtie-bio.sourceforge.net/manual.shtml#example-9--a--m-3---best---strata
Command line: `./bowtie -a -m 3 --best --strata -v 2 e_coli --suppress 1,5,6,7 -c ATGCATCATGCGCCAT`
With AlgoRun: Change `Report-all` to on, `Report-m` to 3, `Report-best` to on, `Report-strata` to on, `Align-v` to 2 and `suppress` to 1,5,6,7



9 Publish your algorithm to the AlgoRun website

If you packaged your algorithm with AlgoRun and want to give your algorithm more visibility, do not hesitate to submit it for listing on the AlgoRun website. The AlgoRun website serves as a repository for all computational algorithms that were packaged using AlgoRun: http://algorun.org

To submit your algorithm for listing, fill the form located at http://algorun.org/submit-algorithm.html