Watchdog

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1 Introduction

Here, we present Watchdog, a WMS for the automated and distributed analysis of large-scale experimental data. Watchdog is implemented in Java and is thus platform-independent.

Main features include:

- · straightforward processing of replicate data
- support for distributed computer systems
- remote storage support
- · customizable error detection
- · manual intervention into workflow execution
- a GUI for workflow construction using pre-defined modules
- a helper script for creating new module definitions
- no restriction to specific programming languages
- · provides a flexible plugin system for extending without modifying the original sources

2 Install and Configure Watchdog

2.1 Requirements

Watchdog is platform independent as it is written in Java and requires JRE (Java Runtime Environment) 1.8 or higher (the GUI is build on JavaFX that is currently not part of most OpenJDK builds). Most of the modules that are delivered with Watchdog require a unix based system and were tested on SUSE Linux. They might not run without any changes on other unix systems or Windows but users can define custom modules that are compatible with their installed software and operating system. Each of the modules might require additional software to be installed. These requirements can be checked for the modules that are delivered with Watchdog with the help of helper scripts/dependencyTest.sh as described below.

2.2 Installation

The installation of Watchdog is very easy. Simply extract the provided archive into a folder of your choice using tar xfvz watchdog.tar.gz The folder must be accessible for remote or cluster executors if you plan to use some.

Alternatively Watchdog can be installed automatically via conda using conda install -c bioconda watchdog-wms. In that case be binaries are named watchdog-cmd and watchdog-gui while the rest of the files is located in \${PREFIX}/share/watchdog-wms-\${VERSION}. If you want to use Watchdog with Docker, read section 7.

In the next few lines the content of each folder is explained:

- core lib: some core functions that can be used in bash module scripts
- doc: contains Watchdog's documentation in html-format
- examples: contains the examples that are also presented in the documentation
- helper_scripts: scripts for generating new modules, configure the examples or testing of all modules
- modules: must contain all modules that should be used in workflows
- test data: contains some test data that is used by multiple modules
- tmp: is used for Watchdog's temporary files
- webserver data: data which is accessed by the internal webserver
- xsd: definition of the module and workflow in xsd format

To test if all software required by installed modules that call bash scripts is available the script hetendencyTest.sh can be executed. It checks if all requirements are installed that are also enforced by the module itself. Only dependencies that are defined in the bash script itself stored in the variable named <a href="mailto:susepi_su

In order to test if all modules that provide tests work as expected on your system you can

run helper_scripts/moduleTest.sh. If you want to test the examples which are discussed in this manual, you can configure them by running:

```
helper_scripts/configureExamples.sh -i /path/to/install/folder/of/watchdog [-m your@mail-adress.com] (mail attribute (-m) is optional)
```

Afterwards the configured examples will be located in /path/to/install/folder/of/watchdog/examples/ and can be executed (from the watchdog installation directory) using the following command: ./watchdog.sh.-x examples/filename.xml or alternatively java -jar jars/watchdog.jar -x examples/filename.xml

```
For instance: ./watchdog.sh -x examples/workflow1_basic_information_extraction.xml
```

If you want to use the workflow designer (GUI), you can start it by using (from the watchdog installation directory): ./workflowDesigner.sh or alternatively java -jar jars/WatchdogDesigner.jar

2.3 E-Mail Server Configuration

As Watchdog will send e-mails it needs a working mail configuration. If you don't want Watchdog to send e-mails, simply don't use the mail attribute of the <tasks> tag. In that case the content of the mails with be printed to the standard output stream.

By default a server listening on SMTP port 25 is expected that accepts mails without authentication. In order to use another configuration the parameter <code>-mailConfig</code> of Watchdog can be used. It expects a tab-separated file that contains information on how to connect to the mail server using the SMTP protocol. If the mail server expects some authentication we strongly suggest to use a mail account that was explicitly created for the use with Watchdog as the password is stored unencrypted.

Example 1: Example mail config for a gmail account

```
mail.smtp.auth true
mail.smtp.host smtp.googlemail.com
mail.smtp.port 587
mail.smtp.user johns_watchdog@gmail.com
mail.smtp.pw r9x741(klsab
mail.smtp.from johns_watchdog@gmail.com
mail.smtp.starttls.enable true
```

Example 1 shows a configuration for a gmail account. More information about the variables that can be used can be found here. An template mail config file that can be edited can be found in examples/mail_config once the examples are configured as described above.

2.4 SSH Configuration

Watchdog supports execution of tasks via ssh on remote hosts. In order to use that feature a private ssh key must be provided. It is strongly recommended that the private key is protected by a passphrase. In that case the passphrase must be entered after Watchdog was started and will be hold encrypted in memory until the passphrase is needed.

A key pair that can be used for ssh authentification can be generated using the tool <u>ssh-keygen</u> that is part of <u>openssh</u>. If you need further information you can find many online tutorials that explain how to use a private key for ssh authentication. E.g. <u>How To Set Up SSH Keys</u> and <u>SSH/OpenSSH/Keys</u>

2.5 Cluster Configuration

Watchdog supports cluster solutions which provide a *DRMAA* java binding. By default it is bundled with a DRMAA binding for the *sun grid engine* (SGE 6.1).

The following environment variables must be set correctly in order to communicate with the SGE:

- SGE ROOT: path to the installation folder of the SGE
- LD_LIBRARY_PATH: path to the library path of the SGE; in most cases it will be \$SGE ROOT/lib/lx24-amd64 or \$SGE ROOT/lib/lx24-x86

Basically there are two ways to change the default cluster extension in order to use another DRMAA solution than the SGE:

- dynamically by adding arguments to the jar invocation:
 - set class name of DRMAA Sessionfactory via -Dorg.ggf.drmaa.SessionFactory=classname
 - 2. add DRMAA java binding to class path via -cp

```
/path/to/drmaaImplementation.jar
```

- permanently by changing Watchdog's jar file:
 - 1. jar files can be opened and edited with every tool that supports zip files
 - 2. replace name of DRMAA Sessionfactory stored in /META-INF/services/org.ggf.drmaa.SessionFactory
 - 3. add class files of the DRMAA java binding to Watchdog's jar file

Probably further settings are needed which depend on the used DRMAA library.

3 Watchdog Overview

3.1 Modules

Modules represent re-usable components that perform certain tasks, e.g. compression of files or creating histograms. Watchdog is delivered with a set of predefined modules. Additionally the user has the possibility to define own modules as described in section 5. The modules are stored in the *modules* directory located in the root folder of the Watchdog installation. Each module is stored in its own folder and consists at least of an XSD file with the name of the module. The XSD file contains a definition of the parameters which can be set in the XML format and the tools which are executed in the background when the module is used.

Example 2: XSD definition of the sleep module

```
<?xml version="1.0" encoding="UTF-8" ?>
 1
     <x:schema xmlns:x="http://www.w3.org/2001/XMLSchema"</pre>
xmlns:vc="http://www.w3.org/2007/XMLSchema-versioning"
vc:minVersion="1.1" xmlns:xerces="http://xerces.apache.org">
 3
 4
           <!-- definition of the task parameters -->
           <x:complexType name="sleepTaskParameterType">
 6
                \langle x:all \rangle
 7
                      <x:element name="wait" type="paramWait sleep"</pre>
minOccurs="1" maxOccurs="1" />
                </x:all>
 9
           </x:complexType>
10
11
12
13
           <!-- make task definition available via substitution
group -->
           <x:element name="sleepTask" type="sleepTaskType"</pre>
substitutionGroup="abstractTask" />
15
16
           <!-- module specific parameter types -->
17
           <x:complexType name="paramWait sleep">
18
                <x:simpleContent>
19
                      <x:restriction base="paramString">
20
                            <x:assertion test="matches($value,</pre>
'(\{[A-Za-z]+\})|(\{(.+))|([[(\{](\{[A-Za-z]+(,s*)\{0,1\})\{0,1\}([0-x]))\})|
9]+(,S^*)\{0,\overline{1}\}\{0,1\}[]\}\})') or matches ($\frac{1}{2}\text{value}, \frac{1}{2}\text{[0-9]+[smhd]}
{0,1}$')" xerces:message="Parameter with name '{$tag}' must match
[0-9]+[smhd]\{0,1\}." />
21
                      </x:restriction>
22
                 </x:simpleContent>
23
           </x:complexType>
```

```
24
25 </x:schema>
```

Example 2 shows parts of the XSD definition of a module which are important to know for the user. At the beginning parameters and flags which are accepted by the module are defined in an element named <code>sleepTaskParameterType</code> (5-9). In this case only one parameter named <code>wait</code> is defined that must occur exactly once (7). The type of the parameter is specified at the bottom of the example (17-23). In this case the parameter is a string that must match a regex pattern, which first accepts numbers followed by a letter as optional suffix (19-21). Additionally values that are placeholders for constants or variables are allowed by the first <code>matches()</code> function whereby the user must take care that the replaced value is valid with regard to the second part of the specification (20). The attribute <code>name</code> of the element in line 14 defines how the module can be referenced in the XML file. In this example the module can be called using the name <code>sleepTask</code>.

3.2 Basic XML structure

Tasks which should be executed by Watchdog must be defined in an XML file. In the following the structure of the XML file is presented. The expression <?Task> is used to refer to a task which is not further specified. In general this syntax is used if some attributes are valid for all classes that inherit from that class type. Within the following examples these variables are user-specific and contain therefore no concrete values:

```
{%INSTALL%} - path to the root installation directory of Watchdog {%MAIL%} - email adress of the user {%EXAMPLE DATA%} - path to the folder in which the example data is located
```

You already have configured your examples by calling the script helper_scripts/configureExamples.sh as described in 2.

Example 3: Most basic XML input for Watchdog

```
<?xml version="1.0" encoding="UTF-8"?>
 1
     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-</pre>
instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
 3
          <!-- begin task block and use that mail to inform the
user on success or failure -->
          <tasks mail="{%MAIL%}">
 6
 7
               <!-- definition a simple sleep task -->
 8
               <sleepTask id="1" name="sleep">
 9
                    <parameter>
                          <wait>30s</wait>
10
11
                    </parameter>
12
               </sleepTask>
```

Example 3 shows a most basic XML file that contains only a single task named <code>sleep</code>. Every XML file that should be parsed by Watchdog must contain a <code><watchdog></code> element as root element (2). The attribute <code>watchdogBase</code> of it must refer to the folder in which Watchdog was installed. The attribute <code>isTemplate</code> prevents Watchdog from executing workflows that contain variables that must be set by the user and is removed automatically by the configure script. Afterwards as childs of <code><tasks></code> the tasks which should be executed must be defined (5). Each task must contain an <code>id</code> and <code>name</code> attribute (8). With the <code><parameter></code> element, values can be assigned to the parameters of the task, which have to be specified in the XSD file of the module. Flags are activated by using <code><flagName>true</flagName></code> or <code><flagName>1</flagName></code> while parameters can be set with <code><paramName>value</paramName></code> (10).

| element | attribute | type | function | |
|-----------------------|----------------|---------|---|--|
| <watchdog></watchdog> | watchdogBase | string | path to the install path of watchdog | |
| <watchdog></watchdog> | isTemplate | boolean | prevents Watchdog from executing unconfigured workflow templates; default: false | |
| <tasks></tasks> | [mail] | string | mail which is used for notification; if not set, the content of the mails with be printed to the standard output stream; default: not set | |
| <tasks></tasks> | [projectName] | string | name of the complete process; default: not set | |
| Task | [id] | integer | numeric id of the task; if not set all id's will be automatically generated; default: not set | |
| Task | name | string | name of the task | |
| Task | [processBlock] | string | processBlock as source of varying parameters (see 4.1) | |
| Task | [executor] | string | execution environment on which the task is executed (see <u>4.3</u>) | |
| Task | [environment] | string | use globally defined environment variables (see 4.5) | |
| Task | [maxRunning] | integer | maximal number of simultaneously running tasks; default: not restricted | |
| Task | [notify] | enum | notification of the user via mail on success; enabled: release complete task at once when all subtasks are finished; subtask: release every subtask separately; default: disabled (see 4.6) | |
| Task | [checkpoint] | enum | does not schedule tasks which depend on this task until manually released by the user; enabled: release complete task at once when all subtasks are finished; subtask: release every subtask separately; defaudisabled | |
| Task | [confirmParam] | enum | allows the user to modify the parameters before the task is scheduled; enabled: task will not be scheduled until the user checks the parameter; default: disabled | |
| Task | [version] | integer | version of the module that should be used for that task; default: 1 (see 5.6) | |
| Task | [posX] | integer | x coordinate for display in GUI; default: not set | |
| Task | [posY] | integer | y coordinate for display in GUI; default: not set | |

In the following sections the structure of the XML format is described in greater detail.

4 Detailed XML format explanation

In the following sections the complete range of functions of Watchdog's XML format is explained. The following elements must be defined as child elements of the <settings> element before the <tasks> element begins and are valid within the complete XML file:

- cessBlock> process a task with varying parameters (see 4.1)
- <executors> define different executor environments (see 4.3)
- <constants> defines constants that substitute placeholders (see 4.4)
- <environments> define or update environment variables (see 4.5)
- <modules> define multiple module include directories (see 4.10)

Apart from the cameter> element, the following elements are allowed in <?Task>

- <environment> define or update environment variables (see 4.5)
- <dependencies> define dependencies between tasks (see 4.2)
- <streams> define location of standard streams and set a working directory (see 4.7)
- <checkers> usage of custom success or error checkers (see 4.11)
- <actions> define task actions that are performed before or after tasks execution (see 4.8)

4.1 Process blocks

Watchdog is able to process multiple tasks of the same type, which differ only in some parameter values, without the need to define all of these tasks separately. This function is referred to as **process blocks** while the tasks created by an process block are called **subtasks** of the task. There are four different possibilities to define process blocks as childs of the **processBlock** element:

- processSequence> argument is numeric
- cprocessFolder> argument is a path to a file
- cessInput> multiple arguments obtained from dependencies
- cessTable> multiple arguments stored in a tab-separated file with names of
 variables stored in the first line

When the cessBlock> attribute of a task is set the argument of the process folder
or sequence is substituted at run time within cpredictions> and <environment> elements in the following manner:

- cessSequence> []/{}/() -> number
- cprocessFolder> {} -> absolute path to the file
- cessFolder> () -> absolute path to the parent folder of the file
- cessFolder> [] -> name of the file
- $< processFolder > [n]/{n} -> n$ suffixes of the filename are truncated using . as separator

- cessFolder> (n) -> n suffixes of the parent folder are truncated using / as
 separator
- $cessFolder> ([{n,sep}]) -> suffixes of the value are truncated using sep as separator (might also be a regex)$
- column named
 \$COL NAME

 ([{\$COL_NAME}]) -> value stored in the column named
- ([{\$COL_NAME, n, sep}]) -> value stored in the column named
 \$COL_NAME but with suffix truncation as described above
- color="block">
- ([{\$RET_NAME, n, sep}]) -> return value of a dependency with the

 name \$RET_NAME\$ but with suffix truncation as described above

If a task depends on two tasks, which return variables with the same name, the return value of the task with the smaller id will be overwritten. Deviating from this, return values from separate dependencies will overwrite the ones from global dependencies if both use the same name for a variable.

Example 4: Definition of different process blocks

```
<?xml version="1.0" encoding="UTF-8"?>
 1
     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-</pre>
instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
 3
 4
          <settings>
              <!-- definition of different process blocks -->
 6
               cessBlock>
                    cprocessSequence name="qualities" start="1"
end="9" step="2" />
                    cialFiles" folder="
{%EXAMPLE DATA%}/spec/" pattern="*.spec" />
                    <baseFolder folder="{%EXAMPLE DATA%}/">
 9
10
                         cprocessFolder name="txtFiles"
folder="txt/" pattern="*.txt" />
                         cprocessFolder name="txtFiles"
folder="other txt/" pattern="*.txt" append="true" maxDepth="1" />
                         cprocessFolder name="gzFiles"
folder="txt zipped/" pattern="*.gz" disableExistenceCheck="true"
/>
13
                         cprocessTable name="sleepTable"
table="processTable.input.txt" />
                   </baseFolder>
15
               </processBlock>
16
         </settings>
17
18
         <tasks mail="{%MAIL%}">
19
               <!-- compress all files with *.txt ending in
/some/base/folder/TXT -->
              <gzipTask id="1" name="compress files"</pre>
20
```

```
processBlock="txtFiles" checkpoint="enabled">
21
                    <parameter>
22
                          <input>{}</input>
2.3
                          <output>
{%EXAMPLE DATA%}/txt zipped/[1].gz</output>
                     </parameter>
25
               </gzipTask>
26
27
               <!-- test quality values 1,3,5,7 and 9 -->
               <gzipTask id="2" name="quality test"
processBlock="qualities" checkpoint="subtask">
                    <dependencies>
30
                          <depends>1</depends>
31
                     </dependencies>
32
                     <parameter>
33
                          <input>
{%EXAMPLE DATA%}/txt/txtFile1.txt</input>
34
                          <output>
{%EXAMPLE DATA%}/qualityTest/txtFile1 q[].qz</output>
                          <quality>[]</quality>
36
                    </parameter>
37
                     <environment>
38
                          <var name="QUALITY">{}</var>
39
                     </environment>
40
               </gzipTask>
41
               <!-- sleep tasks which are created based on a
42
process table -->
               <sleepTask id="3" name="table sleep"</pre>
43
processBlock="sleepTable">
                    <dependencies>
                          <depends>2</depends>
45
46
                    </dependencies>
47
                    <streams>
48
                          <stdout>{$OUT, 1}</stdout>
49
                    </streams>
50
                    <parameter>
51
                          <wait>{$DURATION}</wait>
52
                    </parameter>
53
                    <environment>
                          <var name="IMPORTANT ID RAW">
[$IMPORTANT ID]</var>
                          <var
name="IMPORTANT ID CALC">$([$IMPORTANT ID]*3)
56
                     </environment>
57
               </sleepTask>
58
          </tasks>
59
   </watchdog>
```

Example 4 shows three different ways how process blocks can be specified. First a named qualities is defined that creates numbers 1,3,5,7 and 9 (7). In the next line a cessFolder> is defined that will process all files stored in {%EXAMPLE DATA%}/spec that end with .spec (8). The syntax which must be used in the pattern attribute is the same as in bash. If a (9-14).The attribute disableExistenceCheck that is enabled for the of the folder when it is started (12).

The task with id 1 will compress all .txt files in the folders {%EXAMPLE DATA%}/txt {%EXAMPLE DATA%}/other txt and and store them { %EXAMPLE DATA % } / txt zipped (20-25). Whereas, the task with id 2 will compress a file with different quality values (28-40). The compressed files will be stored with prefix the as and used quality as txtFile1 q {%EXAMPLE DATA%}/qualityTest (34). Additionally, an environment variable with the name *QUALITY* is set which also contains the set quality (38). The sleep task at the end of the example shows how the column of a can be used as input (43-57). If the variable is of numeric type it can also be used within simple calculations which are presented in 4.9 (55).

| Table 2: Attributes in the | context of process blocks |
|----------------------------|---------------------------|
| | |

| element | attribute | type | function |
|--|-----------------------------|---------|---|
| ProcessBlock | name | string | is used as reference in the processBlock attribute of a task |
| Task | processBlock | string | name of a ProcessBlock element |
| ProcessBlock | [append] | boolean | if set to true, two or more process blocks of the same type can be merged; supported by processSequence and ProcessFolder; default: false |
| <pre><pre><pre>cessSequence></pre></pre></pre> | start | double | inclusive start of the numeric series |
| <pre><pre><pre><pre><pre><pre><pre><pre></pre></pre></pre></pre></pre></pre></pre></pre> | [step] | double | number that is added until the value is greater than end; default: |
| <pre><pre><pre><pre><pre><pre><pre><pre></pre></pre></pre></pre></pre></pre></pre></pre> | end | double | break condition, might be inclusive |
| <pre><pre><pre>cprocessFolder></pre></pre></pre> | folder | integer | absolute or relative to a <pre><pre><pre><pre><pre><pre><pre>path</pre> to a folder</pre></pre></pre></pre></pre></pre> |
| <pre><pre><pre>cessFolder></pre></pre></pre> | pattern | string | pattern selecting files that should be substituted; syntax as in bash |
| <pre><pre><pre><pre><pre><pre><pre><pre></pre></pre></pre></pre></pre></pre></pre></pre> | [ignore] | string | files matching that pattern will be ignored; syntax as in bash; default: not set |
| <pre><pre><pre><pre><pre><pre><pre><pre></pre></pre></pre></pre></pre></pre></pre></pre> | [disable ExistenceCheck] | boolean | folder must not exist when Watchdog is started; default: false |
| <pre><pre><pre><pre><pre><pre><pre><pre></pre></pre></pre></pre></pre></pre></pre></pre> | [maxDepth] | integer | a positive integer will cause that $maxDepth$ levels of subdirectories are traversed while by default only the parent folder is processed; default: o |
| <pre><basefolder></basefolder></pre> | folder | string | absolute path which is used as prefix before the path of the <pre><pre><pre><pre><pre><pre>cessFolder></pre> is added</pre></pre></pre></pre></pre> |
| <pre><basefolder></basefolder></pre> | [maxDepth] | integer | see description of <pre>cprocessFolder> [maxDepth]</pre> ; if both are set, the value of the <pre>cprocessFolder> element is set</pre> ; default: 0 |
| <pre><pre><pre>cessTable></pre></pre></pre> | table | string | path to a tab-separated file with header; the column names must consist out of [A-Za-z_] |
| <pre><pre><pre><pre><pre><pre><pre><pre></pre></pre></pre></pre></pre></pre></pre></pre> | [disable ExistenceCheck] | boolean | table file must not exist when Watchdog is started; default: false |

| element | attribute | type | function |
|--|---------------|--------|---|
| <pre><pre><pre><pre><pre><pre><pre><pre></pre></pre></pre></pre></pre></pre></pre></pre> | [compareName] | column | name that should be used to compare names of separate dependencies; default: complete line |
| <pre><pre><pre>cessInput></pre></pre></pre> | sep | string | separator which is used to join multiple values of global dependencies together; default: : |
| <pre><pre><pre>cprocessInput></pre></pre></pre> | [compareName] | string | name of return value that should be used to compare names of separate dependencies; default: name of precursor node |

4.2 Dependencies

By default all tasks specified in the XML document are independent from each other. That implies that all tasks are scheduled at the same time if no other constraints exist. It is possible to define dependencies between tasks using the <depends> element that expects as value the id or name of an already defined task. The element must be a child of a <dependencies> element. Without any arguments the task will not be scheduled until all (sub)tasks of the dependencies have finished successfully. By setting the separate argument to true a subtask can depend only on the corresponding subtask the task depends on. This option is only meaningful if both tasks are process block tasks and work on the same input set or a transformed version of it.

Example 5: Definition of dependencies

```
<?xml version="1.0" encoding="UTF-8"?>
     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-</pre>
instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
 3
 4
          <settings>
 5
               <!-- definition of two process folders -->
 6
               cessBlock>
                    <baseFolder folder="{%EXAMPLE DATA%}/">
                         cprocessFolder name="txtFiles"
folder="txt/" pattern="*.txt" />
                         cprocessFolder name="gzFiles"
folder="txt zipped/" pattern="*.gz" disableExistenceCheck="true"
/>
10
                    </baseFolder>
11
               </processBlock>
12
          </settings>
13
          <tasks mail="{%MAIL%}">
14
15
               <!-- definition a simple sleep task -->
               <sleepTask id="1" name="sleep">
16
17
                    <parameter>
18
                         <wait>30s</wait>
                    </parameter>
19
20
               </sleepTask>
21
22
               <!-- compress all files with *.txt ending in
/some/base/folder/TXT -->
```

```
23
               <gzipTask id="2" name="compress"
processBlock="txtFiles">
24
                     <parameter>
25
                          <input>{}</input>
26
                          <output>
{%EXAMPLE DATA%}/txt zipped/[1].gz</output>
27
                     </parameter>
28
                     <!-- dependency definition -->
29
                     <dependencies>
30
                          <depends>1</depends>
31
                     </dependencies>
32
               </gzipTask>
33
34
               <!-- decompress all files with *.gz ending in
/some/base/folder/TXT ZIPPED -->
               <gzipTask id="3" name="decompress"</pre>
processBlock="gzFiles">
36
                     <parameter>
37
                          <input>{}</input>
38
                          <output>
{%EXAMPLE DATA%}/txt decompressed/[1].txt</output>
39
                          <decompress>true</decompress>
40
                     </parameter>
                     <!-- dependency definition -->
41
42
                     <dependencies>
43
                          <depends separate="true" prefixName="</pre>
[1]">2</depends>
44
                     </dependencies>
               </gzipTask>
45
46
          </tasks>
47
     </watchdog>
```

In example 5 a *compress* task with id 2 is defined which depends on the before defined *sleep* task (23-32). Additionally, a task, which will decompress the compressed files immediately after the compression is finished, is defined (35-45). In order to achieve this behavior the **separate** attribute is set to *true* (43). Because the *.txt* ending of the original filename was cropped and a *.gz* ending was added, only the first part of the filename is considered as specified in the *prefixName* attribute (26,43).

| Table 3: Attributes in the context of dependencies | |
|--|--|
| | |

| element | attribute | type | function | |
|-------------------------------|--------------|---------|---|--|
| <dependencies></dependencies> | | | parent of <depends> elements and child of <?Task></depends> | |
| <depends></depends> | | integer | already defined task id on which the task should depend on | |
| <depends></depends> | [separate] | boolean | if set to <code>true</code> each subtask depends only on its corresponding subtask; default: <code>false</code> | |
| <depends></depends> | [keep4Slave] | boolean | if set to true a executor in slave mode will wait until all tasks with that id, which are running on that slave, are finished; only valid for separate dependencies; default: false | |

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| element | attribute | type | function |
|---------------------|--------------|----------|---|
| <depends></depends> | [prefixName] | [[0-9]*] | only meaningful if separate is set to true; defines in which manner the variables of the two process blocks must be equal to each other: []/[0]: complete variables of the subtasks are compared [n]: it is checked if the variable of a subtask begins with the prefix of the finished subtask this task depends on; the first n parts are taken was prefix whereby '.' is used as separator; default: |
| <depends></depends> | [sep] | string | separator which is used together with prefixName; default: . |

4.3 Execution environments

By default the tasks are executed one after the other locally on the host which runs Watchdog. It is possible to define different execution environments using the <executors> element. Possible environments:

- <local> task is executed on the local host
- <remote> task is executed on a remote host using ssh
- <cluster> task is executed on a computer cluster

Example 6: Definition of different execution environments

```
<?xml version="1.0" encoding="UTF-8"?>
     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-</pre>
instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
 3
 4
          <settings>
 5
               <!-- examples of different execution environments
-->
 6
               <executors>
 7
                     <local name="localhost" maxRunning="2" />
                     <cluster name="defaultCluster" default="true"</pre>
memory="1G" queue="short.q" />
                     <cluster name="highPerformanceCluster"</pre>
slots="4" memory="3G" maxRunning="4" queue="short.g" />
                     <remote name="superComputer"</pre>
user="mustermann" host="superComputer"
privateKey="/path/to/private/auth/key" port="22"
disableStrictHostCheck="false" />
11
               </executors>
12
          </settings>
13
          <tasks mail="{%MAIL%}">
14
15
               <!-- execute this task on the localhost -->
16
               <sleepTask id="1" name="sleep"</pre>
executor="localhost">
17
                     <parameter>
18
                          <wait>30s</wait>
19
                     </parameter>
20
               </sleepTask>
```

In example 6 four different execution environments are defined as childs of the <executors> element (6-11). Tasks scheduled on first executor will run on the host on which Watchdog was started (7). The executor with the name defaultCluster is used by default and runs on the short.q queue of the computer cluster (8). The next executor is reserved for high performance tasks because it reserves 4 slots on the cluster with each slot consuming three gigabyte of main memory (9). In order not to occupy the complete computing power the attribute maxRunning is set to four which means that a maximum of four tasks will run simultaneously on that execution environment. In line 10 an example for a remote executor is given which executes tasks via ssh using a host named superComputer.

Afterwards the same sleep task is defined as in the first example and will run on the local executor (16). The other executors can be tested once you adapted them to your local infrastructure (see $\underline{2.4}$ and $\underline{2.5}$).

| Table 4: Attributes in the context of execution environments | | | | | |
|--|--------------------------|---------|--|--|--|
| element | attribute | type | function | | |
| <br Executor> | name | string | is used as reference in the executor attribute of a task | | |
| Task | executor | string | name of a Executor element | | |
| <br Executor> | [environment] | string | environment with that name is used as default environment; default: not set | | |
| <br Executor> | [default] | boolean | defines which execution environment is taken as default; default: false | | |
| <br Executor> | [maxRunning] | integer | number of tasks that can run at the same time; default: not restricted | | |
| <br Executor> | [workingDir] | string | working directory to which the executor switches before task execution; default: /usr/local/storage/ | | |
| <br Executor> | [stickToHost] | boolean | activates slave mode for that executor which means that tasks that depend on each other are executed on the same execution host; default: false | | |
| <br Executor> | [maxSlaveRunning] | integer | number of tasks that can run at the same time on a slave if stickToHost is enabled; default: 1 | | |
| <br Executor> | [pathToJava] | string | path to java binary which is used for slave mode execution; default: /usr/bin/java | | |
| <remote></remote> | user | string | name of the user on the remote host system | | |
| <remote></remote> | host | string | name of the host which should be used for execution; multiple hostnames must be separated by ';' - in that case the maxRunning argument is applied on each host separately | | |
| <remote></remote> | privateKey | string | path the to private ssh auth key; should be protected by a passphrase! | | |
| <remote></remote> | [port] | integer | port which is used for the ssh connection; default: 22 | | |
| <remote></remote> | [disableStrictHostCheck] | boolean | disables the validation of the public key of the host; not recommended!; default: false | | |
| <cluster></cluster> | [slots] | integer | number of cores which are reserved on the computer cluster; default: 1 | | |
| <cluster></cluster> | [memory] | string | memory per slot suffixed with M (megabyte) or G (gigabyte); default: 3000M | | |

| element | attribute | type | function |
|---------------------|--------------------|---------|---|
| <cluster></cluster> | [queue] | string | queue on which the tasks should run on the computer cluster; default: not set |
| <cluster></cluster> | [disableDefault] | boolean | default parameters (slots, memory and queue) are ignored; default: false |
| <cluster></cluster> | [customParameters] | string | additional parameters that are directly passed to the DRMAA system without further processing; default: not set |

4.4 Global constants

A constant can be defined globally using the <const> elements which must be a child of a <constants> element. The parent element itself must be a child of the <settings> environment. Every <const> element must own a unique name which is set with the name attribute. The value of the constant is stored between the opening and closing element tag. \${NAME_OF_CONSTANT}\$ is substituted with the corresponding constant in every attribute or text content. Only the watchdogBase attribute of <watchdog>, the default attribute of <?Executor> and the <id> attribute of <?Task> and within <depends> elements can not be substituted.

Currently, there is one pre-defined constant named *\$ { TMP}* which is substituted within <? **Task>** tags with the working directory of the executor that will execute the task.

Example 7: Definition and use of global constants

```
<?xml version="1.0" encoding="UTF-8"?>
 1
     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-</pre>
instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
 3
 4
          <settings>
 5
               <!-- definition of a constant named WAIT TIME -->
               <constants>
 7
                     <const name="WAIT TIME">30s</const>
 8
                     <const name="FILE NAME">sleep</const>
 9
                     <const name="LOG BASE">/tmp</const>
10
               </constants>
11
          </settings>
12
          <tasks mail="{%MAIL%}">
13
14
15
               <!-- definition a simple sleep task with constant
replacement -->
16
               <sleepTask id="1" name="sleep test">
17
                     <streams>
18
<stdout>${LOG BASE}/${FILE NAME}.out</stdout>
19
                     </streams>
20
                     <parameter>
2.1
                          <wait>${WAIT TIME}</wait>
22
                     </parameter>
```

```
23 </sleepTask>
24 </tasks>
25 </watchdog>
```

In example 7 three constants are defined (6-10). The constant named \${WAIT_TIME} is used as wait time in the sleep task (21). The other two constants are used to construct the standard output file path (18).

| Table 5: Attributes in the context of global constants | | | | | | | |
|--|------|--------|--|--|--|--|--|
| element attribute type function | | | | | | | |
| <constants></constants> | | | parent of <const> elements and child of <settings></settings></const> | | | | |
| <const></const> | name | string | name of the variable that is replaced with <code>\${name}</code> in attributes and text content; only chars out of [A-Za-z_] are allowed as first character followed by [A-Za-z_0-9] in the name; apart from a few exceptions it is allowed everywhere | | | | |
| <const></const> | | | replacement value | | | | |

4.5 Environment variables

PATH variable is important because executable programs are located only in directories defined by that variable. The environment variables which are set on the host running Watchdog can be simply inherited. With help of the <var> element new variables can be defined or updated. The name of the variable must be defined with the name attribute while the value is stored between the opening and closing element tag. The parent element of each <var> element must be a <environment> element which also owns a name attribute. This name attribute is used to link the environment with a task using the environment attribute all tasks possess. It is also possible to define environment variables locally within task definitions. If local and global variables with the same name are set, the local ones override the global variables.

The following environment variables are set by Watchdog by default:

- IS_WATCHDOG_JOB: if module was executed by Watchdog this value is set to 1
- WATCHDOG_CORES: number of reserved cores if task runs on a cluster environment
- WATCHDOG_MEMORY: number of total reserved memory in megabyte if task runs on a cluster environment

```
Example 8: Definition of environment variables
```

```
5
               <!-- definition of a environment -->
 6
               <environments>
 7
                    <environment name="pathEnv">
                          <var name="PATH"</pre>
 8
update="true">~/software/bin</var>
                    </environment>
10
               </environments>
11
          </settings>
12
13
          <!-- begin task block and use that mail to inform the
user on success or failure -->
          <tasks mail="{%MAIL%}">
15
16
               <!-- definition of a simple sleep task using
custom environment variables -->
17
               <envTask id="1" name="env" environment="pathEnv">
18
                    <streams>
19
                          <stdout>/tmp/env.test</stdout>
20
                    </streams>
21
22
                    <!-- definition of a local environment with
two variables -->
23
                    <environment>
24
                          <var name="SHELL">/bin/sh</var>
25
                          <var name="TEST" update="true"</pre>
sep="@">separator test</var>
26
                    </environment>
27
               </envTask>
          </tasks>
28
29
     </watchdog>
```

In example 8 an environment named <code>pathEnv</code> is defined in which the variable <code>PATH</code> is updated (8). The entry <code>~/software/bin</code> is added at the beginning of the <code>PATH</code> variable and after the default seperator character the previous value is kept. The <code>environment</code> attribute of the <code>env</code> task is set to the name of the previously defined environment (17). Additionally two local environment variables are defined (23-26). The first one replaces the default shell with <code>/bin/sh</code> while the second one updates a variable called <code>TEST</code> using an alternative separator.

| Table 6: Attributes in the context of environment variables | | | | |
|---|------------------|---------|--|--|
| element | attribute | type | function | |
| <pre><environment></environment></pre> | name | string | is used as reference in the environment attribute of a task | |
| <environment></environment> | [copyLocalValue] | boolean | copies all environment variables which are set on the host running Watchdog; set variables are not deleted on the remote system; bash functions which names are ending with () are not copied as this might cause problems; default: false | |

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| element | element attribute | | function |
|-----------------------------|--------------------------------|---------|---|
| <environment></environment> | vironment> [useExternalExport] | | uses a external command to set the variables; is necessary to update variables on remote or cluster executors and might also be necessary to set environment variables on remote hosts because of ssh security policies; default: <pre>true</pre> |
| <environment></environment> | [shebang] | string | shebang which is used for the script that first executes the export commands and afterwards the real commands; default: #!/bin/bash |
| <environment></environment> | [exportCommand] | string | custom command to set a environment variable; {\$NAME} and {\$VALUE} are substituted and must be part of the command; default: export {\$NAME} = "{\$VALUE}" |
| Task | environment | string | name of a <environment> element</environment> |
| <var></var> | | string | value of the environment variable |
| <var></var> | name | string | name of the environment variable |
| <var></var> | [update] | boolean | if true the value is added at the beginning of the variable and the old values comes afterwards separated with the value stored in the sep attribute; default: false |
| <var></var> | [sep] | string | separator which is used when the value of the variable should be updated; default: : |
| <var></var> | [copyLocalValue] | boolean | copies the environment variables with the name name which is set on the host running Watchdog; default: false |

4.6 Mail notification

By default Watchdog informs the user only when an error occurs during the execution of a task or if an error was detected afterwards. But these behaviour can be changed using the **notify** attribute of tasks.

Example 9: Different mail notification options

```
<?xml version="1.0" encoding="UTF-8"?>
     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-</pre>
instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
 3
 4
          <settings>
 5
               <!-- definition of different process blocks -->
 6
               cessBlock>
                    cprocessSequence name="sleepTime" start="5"
 7
end="15" step="5" />
               </processBlock>
 9
          </settings>
10
          <!-- begin task block and use that mail to inform the
user on success or failure -->
12
         <tasks mail="{%MAIL%}">
13
               <!-- definition a simple sleep task -->
               <sleepTask id="1" name="sleep simple"</pre>
14
notify="enabled">
15
                    <parameter>
16
                          <wait>10s</wait>
17
                    </parameter>
```

```
18
                </sleepTask>
19
20
                <!-- definition of process sequence sleep tasks --
>
21
                <sleepTask id="2" name="sleep process sequence"</pre>
notify="subtask" processBlock="sleepTime">
22
                     <parameter>
23
                           <wait>[]s</wait>
2.4
                     </parameter>
25
                </sleepTask>
2.6
          </tasks>
27
     </watchdog>
```

In example 9 different notification options are presented. The first defined task is the simple sleep task from the previous examples for which the **notify** attribute is set to **enabled** (14). Once the task is finished a mail will be sent to the address the user specified in the **mail** attribute of the **<tasks>** element (12). The second defined task is based on a process block named **sleepTime** and causes Watchdog to inform the user as soon as a subtask is finished because the **notify** attribute is set to **subtask** (7, 21).

| Table 7: Attributes in the context of mail notification | | | | |
|---|--------------|--------|---|--|
| element | attribute | type | function | |
| <tasks></tasks> | mail | string | mail adress which is used for notification | |
| Task | notify | enum | enabled: inform when complete task was executed subtask: inform when a subtask was executed disabled: notification only in case of an error | |
| Task | processBlock | string | reference to a process block when notify is set to subtask | |

4.7 Standard streams and working directory

By default the stdout and stderr stream of the tool which is executed by watchdog is not saved. This can be changed by setting a path via the <stdout> or <stderr> element. It is also possible to use a file as input via the <stdin> element. Additionally, a working directory can be set by using the <workingDir> element. When this is done also relative path for <stdout>, <stderr> and <stdin> are allowed. Other than usual, the elements must occour in the same order as they are listed in the following: <workingDir>, <stdout>, <stderr> and <stdin> (but each of them is optional)

Example 10: Definition of standard streams and working directory

```
1     <?xml version="1.0" encoding="UTF-8"?>
2     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
3
4          <!-- begin task block and use that mail to inform the user on success or failure -->
```

```
5
          <tasks mail="{%MAIL%}">
 6
 7
               <!-- definition a simple sleep task -->
 8
               <sleepTask id="1" name="sleep">
 9
                    <parameter>
                         <wait>30s</wait>
10
11
                    </parameter>
                    <!-- definition of a standard output location
12
and switch of the working directory -->
13
                   <streams>
14
                         <workingDir>/tmp/</workingDir>
15
                         <stdout>
{%EXAMPLE DATA%}/sleepTest.out</stdout>
16
                         <stderr
append="true">sleepTest.err</stderr>
17
                    </streams>
18
               </sleepTask>
19
          </tasks>
20
     </watchdog>
```

In example 10 the working directory is set to /tmp (14). Afterwards, the standard output of the sleep task is written to the file ${\ensuremath{\mbox{\it EXAMPLE_DATA}\mbox{\it BleepTest.out}}\mbox{\it (15)}$. The standard error stream is appended at the end of a file named /tmp/sleepTest.err (16).

| element | attribute | type | function |
|---------------------------|-----------|------|---|
| <streams></streams> | | | saves used resources to .res if standard output stream is saved to a file; default: false |
| <workingdir></workingdir> | | | sets a custom working directory before the tool is executed; default: /usr/local/storage |

Table 8: Attributes in the context of standard streams and working directory

| (Streams/ | | Doolean | saved to a file; default: false |
|-------------------------------------|-------------------------|---------|--|
| <workingdir></workingdir> | | string | sets a custom working directory before the tool is executed; default: /usr/local/storage |
| <stdout></stdout> | | string | writes standard output stream into file; default not saved |
| <stderr></stderr> | | string | writes standard error stream into file; default not saved |
| <stdin></stdin> | | | file is used as standard input; default: not set |
| <stdin></stdin> | [disableExistenceCheck] | boolean | file must not exist when Watchdog is started; default: false |
| <stdout>/<stderr></stderr></stdout> | [append] | boolean | appends the stream at the end of the file; default: false |

4.8 Task actions

Additional operations can be executed before and after the actual task is executed. Currently a set of IO operations are implemented that can be used to roll out data the task depends on or to clean up once the task is finished. This feature is especically usefull when Watchdog is running in slave mode (see 4.3) in order to reduce load for the shared file system as some files might be requirements for different tasks. Hence, these files would have to be transfered multiple times from the shared file system to the host executing the task.

Moreover, files stored on remote files systems can be up- or downloaded by Watchdog.

By default, virtual file systems based on the protocols File, HTTP, HTTPS, FTP, FTPS and SFTP as well as the main memory (RAM) are supported. These virtual file systems are provided by the Commons Virtual File System project of the Apache Software Foundation. Examples for valid URIs of these file systems can be can be found here. However, any file system with an implementation of the FileProvider can also be included by the user as described in 6.1.

Task actions are defined in an <actions> tag as child of <?Task>. Slave mode is automatically activated if a task action is used. Currently six different IO operations are implemented:

- <createFile> creates an empty file
- <createFolder> create an empty folder
- <copyFile> copies a file
- <copyFolder> copies a folder (with content)
- <deleteFile> deletes a file
- <deleteFolder> deletes a folder (with content)

The event after which the task actions are executed must be defined using the time attribute each <actions> tag owns. The following arguments are available:

- beforeTask before the task is executed
- afterTask after the task is executed
- onSuccess when the task was successfully executed
- onFailure when task execution failed
- beforeTerminate before Watchdog or a slave terminates itself

Example 11: Definition of task actions

```
<?xml version="1.0" encoding="UTF-8"?>
     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-</pre>
instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
 3
          <tasks mail="{%MAIL%}">
 5
               <gzipTask id="1" name="gzip task">
 6
                    <parameter>
 7
                          <!-- path to a file that does not exist
yet -->
<input>/tmp/watchdog file to compress.tmp</input>
                    </parameter>
 9
10
                    <!-- action that copies a to the input
location -->
11
                    <actions time="beforeTask">
                          <copyFile file="</pre>
{%INSTALL%}examples/example task actions.xml"
destination="/tmp/watchdog file to compress.tmp" override="true"
/>
```

In example 11 a file name /tmp/watchdog_file_to_compress.tmp is compressed using gzip (5-14). Before the compress task is executed, the task action defined within the <actions> tag is executed because the time attribute is set to beforeTask (11-13). The task action copies the file stored in {%INSTALL%}/examples/example_task_actions.xml to /tmp/watchdog file to compress.tmp (12).

| element | attribute | type | function |
|--|------------------------|---------|---|
| <actions></actions> | time | enum | defines when the task action block is executed; before Task: before the task is executed; after Task: after the task is executed; on Success: when the task was successfully executed; on Failure: when task execution failed; before Terminate: before Watchdog or a slave terminates itself |
| <actions></actions> | [uncoupleFromExecutor] | boolean | if enabled, task actions are executed on the host running Watchdog instead of the execution host; default: false |
| <createfile></createfile> | file | string | path to the file that should be created |
| <createfile></createfile> | [override] | boolean | defines if an existing file should be overwritten; default: fals |
| <createfile></createfile> | [createParent] | boolean | defines if the parent directories should be created if nonexistent; default: true |
| <pre><createfolder></createfolder></pre> | folder | string | path to the folder that should be created and will be empty if action succeeds |
| <pre><createfolder></createfolder></pre> | [override] | boolean | defines if an existing folder should be deleted; default: false |
| <pre><createfolder></createfolder></pre> | [createParent] | boolean | defines if the parent directories should be created if nonexistent; default: true |
| <copyfile></copyfile> | file | string | path to the file that should be copied |
| <copyfile></copyfile> | destination | string | path to the destination of the new file |
| <copyfile></copyfile> | [override] | boolean | defines if an existing file should be overwritten; default: fals |
| <copyfile></copyfile> | [deleteSource] | boolean | deletes the source file after the copy operation; default: false |
| <copyfile></copyfile> | [createParent] | boolean | defines if the parent directories should be created if nonexistent; default: true |
| <copyfolder></copyfolder> | folder | string | path to the folder that should be copied |
| <copyfolder></copyfolder> | destination | string | path to the destination folder |
| <copyfolder></copyfolder> | er> [pattern] | | pattern selecting files that should be copied in that folder; syntax as in bash |
| <copyfolder></copyfolder> | [override] | boolean | defines if an existing folder should be deleted; default: false |
| <copyfolder></copyfolder> | [deleteSource] | boolean | deletes the source folder after the copy operation; default: false |
| <copyfolder></copyfolder> | [createParent] | boolean | defines if the parent directories should be created if nonexistent; default: true |
| <deletefile></deletefile> | file | string | path to the file that should be deleted |
| <deletefolder></deletefolder> | folder | string | path to the folder that should be deleted |

| element | attribute | type | function |
|-------------------------------|-----------|---------|--|
| <deletefolder></deletefolder> | [pattern] | ESHIIIG | pattern selecting files that should be deleted in that folder; syntax as in bash |

4.9 Simple calculations

Within a <?Task> element simple calculations can be preformed using the \$(expr)\$ construct whereby expr must be a numerical equation. The following operators are supported: +, -, *, /, ^, 2 and 3. Additional the brackets () are provided. Moreover in case of a processSequence> i is replaced by the current value of the process sequence. In the more general case of a processBlock> x is substituted by an increasing number starting at 1. The result of all calculations is rounded to five decimal places or converted to an integer if it is one.

Example 12: Definition of simple calculations

```
<?xml version="1.0" encoding="UTF-8"?>
 1
     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-</pre>
instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
 4
          <settings>
 5
               <!-- definition of two process blocks -->
 6
               cessBlock>
                    cprocessSequence name="sleepTime" start="1"
end="5" step="1.5" />
                    cprocessFolder name="txtFiles" folder="
{%EXAMPLE DATA%}/txt/" pattern="*.txt" />
               </processBlock>
10
          </settings>
11
          <tasks mail="{%MAIL%}">
12
13
               <!-- sleep task with a simple calculation -->
14
               <sleepTask id="1" name="sleep"</pre>
processBlock="sleepTime">
15
                    <parameter>
16
                          <wait>$((i+1)^2-1)s</wait>
17
                    </parameter>
18
               </sleepTask>
19
20
               <!-- compress txt files and write log files to
()/log/* -->
               <gzipTask id="2" name="quality test"
processBlock="txtFiles">
2.2
                    <streams>
23
                          <stdout>()/log/$(x).out</stdout>
24
                    </streams>
25
                    <parameter>
26
                          <input>{}</input>
27
                          <output>{}.gz</output>
```

In example 12 the usage of the \$(expr)\$ construct is shown. The wait time for the sleep task is calculated based on the input numbers of the processSequence>(7, 16). In the second gzip task the number of the subtask is used to name the standard output files (23).

4.10 Multiple module search folders

By default Watchdog tries to locate modules in a folder named <code>modules/</code> stored in the installation directory of Watchdog. By using the <code><modules></code> element as child of <code><settings></code>, additional folders can be added.

Example 13: Definition of multiple module include folders

```
<?xml version="1.0" encoding="UTF-8"?>
     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-</pre>
instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
 3
 4
          <settings>
               <!-- TODO: modify one of these folders
{%INSTALL%}myCustomFolder/ or -->
               <!-- /home/TODO/additionalModules/ to match a
folder that contains the 'sleep' module -->
 7
               <modules defaultFolder="myCustomFolder/">
<folder>/home/TODO/additionalModules/</folder>
               </modules>
10
          </settings>
11
          <!-- begin task block and use that mail to inform the
user on success or failure -->
          <tasks mail="{%MAIL%}">
13
14
               <!-- definition a simple sleep task -->
               <sleepTask id="1" name="sleep">
15
16
                    <parameter>
17
                         <wait>30s</wait>
18
                    </parameter>
19
               </sleepTask>
20
          </tasks>
2.1
     </watchdog>
```

In example 13 the default directory is changed to <code>myCustomFolder/</code> with the <code>defaultFolder</code> attribute (7). Moreover, in line 8 an additional folder is added to Watchdog's search path. Watchdog will now try to locate modules in the directories <code>{%INSTALL%}/myCustomFolder/</code> and <code>/home/additionalModules/</code>. In order to test that example you must create a new folder, copy the <code>sleep</code> module from Watchdog's module folder and adapt the path in line 7 or 8 to match that folder.

| Table 10: Attributes in the context of module include_folders | | | | |
|---|-----------------|--------|---|--|
| element | attribute | type | function | |
| <modules></modules> | [defaultFolder] | string | changes the default search folder; an absolute or relative path to Watchdog's install dir is allowed (must end with /); default: modules/ | |
| <folder></folder> | | string | adds a new directory to that is used for localization of modules | |

4.11 Custom success and error checker

In some cases the exit code of a command is not a reliable indicator whether the command was executed successfully or not. For example some tools return as exit code zero regardless of whether the command succeeded or failed. Furthermore, a command could succeed technically but the desired result is not obtained (e.g. wrong index used for mapping of RNA-seq data results in a very low mapping rate). In order to handle such cases the user has the option to implement custom success and error checkers in Java that are executed by Watchdog once a task has terminated. Two steps must be performed to use custom checkers: implementation in Java and invocation in the XML workflow.

Interfaces for checkers are stored in the package *de.lmu.ifi.bio.watchdog.interfaces*. Basically a function returning a boolean value that indicates whether the task succeeded or failed must be implemented. The constructor must accept as first argument a object of the type *Task* that contains information about the task that was finished. Additional arguments of type *Boolean*, *Integer*, *Double* or *String* can be passed via the XML definition.

Example 14: Load custom checkers

```
1
     <?xml version="1.0" encoding="UTF-8"?>
     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-</pre>
instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
 3
 4
          <!-- begin task block and use that mail to inform the
user on success or failure -->
 5
          <tasks mail="{%MAIL%}">
 6
 7
               <!-- definition a simple sleep task -->
 8
               <sleepTask id="1" name="sleep">
 9
                    <parameter>
                          <wait>30s</wait>
10
11
                    </parameter>
```

```
12
                    <checkers>
13
                          <!-- load a success checker with one
additional constructor argument -->
                          <!-- it will check, if the file
{%INSTALL%}examples/mail config exists and is not empty -->
                          <checker classPath="</pre>
{%EXAMPLE DATA%}/OutputFileExistsSuccessChecker.class"
className="de.lmu.ifi.bio.watchdog.successChecker.OutputFileExist$$
type="success">
                               <cArg type="string">
{%INSTALL%}examples/mail config</cArg>
                          </checker>
18
                    </checkers>
19
               </sleepTask>
20
          </tasks>
21
     </watchdog>
```

Example 14 shows an example of how an success checker can be added to a task by using the <checkers> element as a child of <?Task> (12-18). In addition to the location of the compiled Java class and the full class name arguments can be passed to the constructor of the class. In this example one variable of type string is passed to the constructor of the success checker using the <carg> element (16). Once the task is finished, the checkers are evaluated in the same order as they were added in the XML workflow. In cases in which simultaneously success and error were detected, the task will be treated as failed. In this example the success checker will ensure that the file {%INSTALL%}/examples/mail config exists and is not empty (15-16)

| Table 11: Attributes in the context of custom checkers | | | | |
|--|-----------|--------|--|--|
| element | attribute | type | function | |
| <checker></checker> | type | enum | type of the checker; success: checker should be used as success checker; error: checker is used as error checker | |
| <checker></checker> | className | string | complete class name including the package the class is located in | |
| <checker></checker> | classPath | string | absolute path to the compiled java class file | |
| <carg></carg> | type | enum | type to which the argument should be parsed in java; possible values: boolean, integer, double and string | |

5 Creating custom modules

In the following the steps that are needed to create a custom module named nameOfModule are explained. Basic XSD skills are needed to understand how things work together. Modules are defined in XSD format and should have the basic structure showed in example 15. To actually create modules the script helper_scripts/createNewModule.sh can be used and modified by hand as not all settings can be configured by it.

As a first step, a folder with the name <u>nameOfModule</u> must be created in the <u>modules</u> folder. That folder must contain a file named <u>nameOfModule.xsd</u> which will hold the actual module definition.

5.1 Input parameter definition

Example 16 shows how input parameters and flags can be defined.

In line 4 and 5 two parameters are defined while line 6 creates a flag. Using the minOccurs and maxOccurs attributes it can be specified how often a parameter can be

used. Also parameters can have different types which are enforced during the validation of the XML workflows. Some pre-defined types are

- paramBoolean (for flags)
- paramString
- paramInteger
- paramDouble

These types accept by default booleans, strings, integers or doubles but also allow all values that are substituted by Watchdog. Moreover own parameter types can be defined as showed in example 17.

Example 17: Input parameter 1 <!-- module specific parameter types --> <x:complexType name="paramWait sleep"> 3 <x:simpleContent> <x:restriction base="paramString"> <x:assertion test="matches(\$value, '(\${[A-Za-</pre> $z]+\}) | (\$(.+)) | ([[({](\$[A-Za-z]+(,s*){0,1}){0,1}}([0-9]+(,S*)$ $\{0,1\}$) $\{0,1\}$ []) $\}$]) ') or matches $(\text{value}, '^[0-9]+[\text{smhd}] \{0,1\}$ $\}$ ')" xerces:message="Parameter with name '{\$tag}' must match [0-9]+ $[smhd] \{0,1\}." />$ 6 </x:restriction> 7 </x:simpleContent> 8 </x:complexType>

5.2 Output parameter definition

Optionally a module can return output parameters that can be used for the following tasks as input. Return parameters must be written to a file in the format {%VAR_NAME%} TAB {%VALUE%}. The name of the file to write into is automatically sent to the module by Watchdog using the returnFilePathParameter parameter. If you want to change this default parameter name see <u>5.3</u>.

Example 18: Output parameter

```
9 </x:complexContent>
10 </x:complexType>
```

Line 6 in example 18 specifies that the module must return a parameter named <code>outputParam1</code> of type <code>x:string</code>. The module itself must ensure that the parameters are written physically before the module exits or otherwise Watchdog will terminate itself. In case of a bash script which is executed, two functions named <code>writeParam2File</code> and <code>blockUntilFileIsWritten</code> defined in <code>core lib/functions.sh</code> can be used.

5.3 Binary call command and other settings

Now the command that will be executed can be defined. Example 19 specifies that a script named <code>nameOfModule.sh</code> that is stored in <code>modules/nameOfModule</code> will be called.

In addition to that, the following settings can be modified:

- binName: name of the command which should be called
- preBinCommand: command that is added before the binName; e.g. interpreter
- *isWatchdogModule*: by default the command must be located in modules/*binName*; if this parameter is false the command must point to a absolute binary or be reachable via the PATH environment variable
- returnFilePathParameter: name of the parameter that is used to store the return values
- watchdogModuleVersionParameter: name of the parameter that passes the module version to the called command if a version different to 1 should be used; default: moduleVersion (using the default parameter pasing options defined with the settings below; use an empty string to disable the passing of the module version)
- paramFormat: defines how names of parameters are prefixed; (do not print parameter name, or --); default: --
- spacingFormat: defines how names of parameters and values are spaced; default:
 blank
- quoteFormat: defines how values are quoted; default: single quoting

• separateFormat: defines the separator string between multiple occurrences of the
same parameter; default: ,

The last three arguments can also be used for each parameter separately.

5.4 Assign a name to the new module

Finally, a name must be assigned to the module. This can simply be done by creating a element with the attribute **name** of type <code>nameOfModuleType</code> and **substitutionGroup** set to <code>abstractTask</code>. Example 20 shows the needed line for the example module. Afterwards the type of the task is defined (5-15). If no output parameters are used line 10 can be omitted.

```
Example 20: Assign a name to the module
 1
     <!-- make task definition availible via substitution group -
->
     <x:element name="nameOfModuleTask" type="nameOfModuleType"</pre>
substitutionGroup="abstractTask" />
     <!-- definition of final task -->
 4
 5
     <x:complexType name="nameOfModuleTaskType">
           <x:complexContent>
 7
                <x:extension base="nameOfModuleTaskOverrideType">
 8
                      \langle x:all \rangle
 9
                           <x:element name="parameter"</pre>
type="nameOfModuleTaskParameterType" minOccurs="1" maxOccurs="1"
/>
10
                           <x:element name="return"</pre>
type="nameOfModuleTaskReturnType" minOccurs="0" maxOccurs="0" />
                           <x:group ref="defaultTaskElements" />
11
12
                      </x:all>
13
                </x:extension>
           </x:complexContent>
14
15
     </x:complexType>
```

5.5 Putting it all together

Example 21 shows the definition of the complete module.

Example 21: Putting it all together

```
1     <?xml version="1.0" encoding="UTF-8" ?>
2          <x:schema xmlns:x="http://www.w3.org/2001/XMLSchema"
xmlns:vc="http://www.w3.org/2007/XMLSchema-versioning"
vc:minVersion="1.1" xmlns:xerces="http://xerces.apache.org">
3
```

```
4
          <!-- definition of the task parameters -->
 5
          <x:complexType name="nameOfModuleTaskParameterType">
                <x:all>
                     <x:element name="parameter1"</pre>
type="paramAbsoluteFilePath" minOccurs="1" maxOccurs="1" />
                     <x:element name="parameter2"</pre>
type="paramString" minOccurs="0" maxOccurs="unbounded" />
                     <x:element name="flag1" type="paramBoolean"</pre>
minOccurs="0" maxOccurs="1" />
                </x:all>
11
          </x:complexType>
12
13
          <!-- define output parameters which must be written to
a file -->
14
          <x:complexType name="nameOfModuleTaskReturnType">
15
                <x:complexContent>
16
                     <x:extension base="taskReturnType">
17
                          <x:all>
18
                                <x:element name="outputParam1"</pre>
type="x:string" />
19
                          </x:all>
20
                     </x:extension>
21
                </x:complexContent>
22
          </x:complexType>
2.3
2.4
          <!-- set command and other settings -->
25
          <x:complexType name="nameOfModuleTaskOverrideType">
26
                <x:complexContent>
27
                     <x:restriction base="baseAttributeTaskType">
28
                          <x:attribute name="binName"</pre>
type="x:string" fixed="nameOfModule.sh" />
29
                     </x:restriction>
30
                </x:complexContent>
31
          </x:complexType>
32
          <!-- make task definition available via substitution
33
group -->
          <x:element name="nameOfModuleTask"</pre>
type="nameOfModuleTaskType" substitutionGroup="abstractTask" />
35
36
          <!-- definition of final task -->
37
          <x:complexType name="nameOfModuleTaskType">
38
                <x:complexContent>
39
                     <x:extension
base="nameOfModuleTaskOverrideType">
40
                          \langle x:all \rangle
41
                                <x:element name="parameter"</pre>
type="nameOfModuleTaskParameterType" minOccurs="1" maxOccurs="1"
/>
42
                                <x:element name="return"</pre>
type="nameOfModuleTaskReturnType" minOccurs="0" maxOccurs="0" />
43
                                <x:group ref="defaultTaskElements"</pre>
```

5.6 Module versions

As parameters of the command that is called by the module might change over time, it is possible to define different versions of the same module. The version that should be used during XML validation and workflow execution can be set using the **version** attribute each <?Task> tag owns. By default version 1 of each module is used. Be aware that only one version of the same module can be used within a workflow.

In order to avoid duplication of the complete XSD file, the minimum and maximum supported module version can be defined for each tag within the XSD file using the minVersion and maxVersion attributes. If a tag is not part of a particular version, it is removed with all its childs from the XSD file that is generated dynamically at runtime for that module version. By using these two attributes the input parameter, the return parameter, the called command and more can be changed for different module version. Example 22 shows a part of the featureCounts module. Among other things a parameter needs to be renamed to support the most recent binary of featureCounts (11-12).

Example 22: Rename of parameters

```
<?xml version="1.0" encoding="UTF-8" ?>
     <x:schema xmlns:x="http://www.w3.org/2001/XMLSchema"</pre>
xmlns:vc="http://www.w3.org/2007/XMLSchema-versioning"
vc:minVersion="1.1" xmlns:xerces="http://xerces.apache.org">
 3
 4
          <!-- definition of the task parameters -->
 5
          <x:complexType name="featureCountsTaskParameterType">
                \langle x:all \rangle
 6
 7
                     <!-- attributes common to all versions -->
 8
 9
                     <!-- attributes that differ between versions
10
-->
11
                     <x:element name="minOverlap"</pre>
type="paramInteger" minOccurs="0" maxOccurs="1" maxVersion="1" />
12
                     <x:element name="minReadOverlap"</pre>
type="paramInteger" minOccurs="0" maxOccurs="1" minVersion="2" />
13
                </x:all>
14
15
          </x:complexType>
```

```
16 ...
17 </x:schema>
```

Example 23 shows how a module script can be made version dependent using bash functions that are delivered with Watchdog. First. the bash variable \${MODULE VERSION PARAMETER NAME} is set to the complete name of the parameter that is used to pass the module version (e.g. --moduleVersion) (3). After sourcing of version automatically includeBasics.sh the module is \$ {MODULE VERSION} variable. This information can be used to alter the parameters and the behavior of the script as an alternative to duplication if differences between module versions are only minor (15,18).

Example 23: Version dependent bash script

```
1
     #!/bin/bash
 2
     SCRIPT FOLDER=$( cd "$( dirname "${BASH SOURCE[0]}" )" &&
pwd )
     MODULE VERSION PARAMETER NAME="--moduleVersion"
     source $SCRIPT FOLDER/../../core lib/includeBasics.sh $@
 5
 7
     # define parameters
     # params used in any version of the module
    DEFINE string 'annotation' '' 'feature annotation in GTF or
 9
SAF format' 'a'
10
     DEFINE string 'input' '' 'index bam file which should be
used for counting' 'i'
     DEFINE string 'output' '' 'path to output file' 'o'
11
12
     . . .
13
     # params only available in module version 1
14
15
     if [ ${MODULE VERSION} -eq 1 ]; then
16
          DEFINE string 'minOverlap' '1' '[optional] minimum
number of overlapped bases required to assign a read to a
feature; also negative values are allowed' 'm'
     # params only available in module version 2
17
18
     elif [ ${MODULE VERSION} -eq 2 ]; then
          DEFINE string 'minReadOverlap' '1' '[optional] minimum
number of overlapped bases required to assign a read to a
feature; also negative values are allowed' 'm'
20
2.1
     fi
     DEFINE integer 'moduleVersion' '1' '[optional] version of
the module that should be used' ''
     DEFINE boolean 'debug' 'false' '[optional] prints out debug
messages.' T'
24
```

5.7 Other matters

Exit codes: The module developer must ensure that a command does only exit with exit status 0 if the command was executed sucessfully. File <code>core_lib/exitCodes.sh</code> contains some exit codes which names are also included in mail notifications if they are used. Custom exit codes can be easily added.

Error messages: Watchdog can detect by default error messages in standard out and standard error streams if they begin with <code>[ERROR]</code>. The errors are only stored if standard out and error files are saved to disk using the <code><streams></code> tag. If an error was detected but the exit code was 0 the command will also fail.

Module test: A script named $test_nameOfModule.sh$ can also be part of the module. It is automatically called, if the user calls $helper_scripts/moduleTest.sh$. Also the module folder might contain some test data in the folder $test_data$. For simple test cases the bash function testExitCode can be used to test, if an input leads to the expected output.

6 Extend Watchdog's functionality

In the following sections two different ways to extend Watchdog's functionality are described.

- Virtual File Systems that can be used within task actions (see 6.1)
- XML Plugins that add new <?Executor> and <?ProcessBlock> elements (see 6.2)

6.1 Virtual file systems for task actions

With the help of task actions, file system operations can be performed before and after tasks (see <u>4.8</u>). By default, virtual file systems based on the protocols File, HTTP, HTTPS, FTP, FTPS and SFTP as well as the main memory (RAM) are supported. These virtual file systems are provided by the Commons Virtual File System project of the Apache Software Foundation.

In order to add a new virtual file system, a class that implements the *VFSRegister* interface can be addded to the jar-file. The class will be automatically loaded by Watchdog and the new virtual file system will be useable without other modifications. The following four methods must be implemented for the interface:

- getFileProvider must return an instance of the FileProvider interface as
 defined in the Commons Virtual File System project
- getURLSchemes returns the url schemes that should be used in combination with that FileProvider (e.g. ftp)
- getMimeTypes sets schemes that should be used for specific mimetypes

The class <code>SimpleVFSRegister</code> can be extended if an instance of the <code>FileProvider</code> class can be created without arguments. Then only the name of the <code>FileProvider</code> class and the URL schemes that should be used must be defined. Example 24 shows how the virtual FTP file system is integrated in Watchdog by using the <code>FtpsFileProvider</code> class of the Commons Virtual File System project.

Example 24: Simple implementation of the VFSRegister interface

```
package de.lmu.ifi.bio.watchdog.task.actions.vfs.impl;

public class FTPSVFSRegister extends SimpleVFSRegister {

private static final String CLASS_NAME =

"org.apache.commons.vfs2.provider.ftps.FtpsFileProvider";

private static final String[] SCHEME = new String[]

ftps"};

public FTPSVFSRegister() throws Exception {
```

6.2 XML Plugins

Watchdog provides a flexible plugin system that allows extending Watchdog by additional types of executors and process blocks without modifying the original Java classes. Essentially, this means creating a new XML element for use in Watchdog workflows as well as implementing additional Java classes that provide the functionality for this element. In brief, you have to do the following to use the plugin system:

- create an XSD file describing the new element and its parent element for use in Watchdog workflows
- Extend a few abstract classes
- Add class files for the new classes to the Watchdog jar-file and copy the new XSD file to a sub-directory of the Watchdog installation directory

In the Watchdog command-line version, all non-abstract classes in the Watchdog jar-file that extend the <code>XMLParserPlugin</code> abstract class are loaded dynamically during workflow execution. Currently, this is restricted to XML parsers for the generic type <code>ProcessBlock</code> or <code>ExecutorInfo</code>. The XML parser for a new XML element provides the functionality to parse this element in a workflow (i.e. a new executor or process block type) and to create a new object representing the corresponding element type. Here, the four most important functions of the <code>XMLParserPlugin</code> abstract class that have to be implemented are:

- getNameOfParseableTag: returns the name of the element the class can parse
- getNameOfParentTag: returns the name of the parent element of this element
- *getXSDDefinition*: returns the path to the XSD file describing this element (relative to the *xsd* sub-directory of the Watchdog directory)
- parseElement: implements the actual parsing process.

The last function creates an object of a class representing the new element. This class has to implement the interfaces <code>XMLDataStore</code> and <code>XMLPlugin</code>, for instance by extending one of the abstract classes <code>ProcessBlock</code> or <code>ExecutorInfo</code> or one of their subclasses.

For use in the Workflow designer GUI of Watchdog, two additional requirements have to be met:

- An FXML file has to be provided describing how the attributes of the new element type are represented graphically. FXML is an XML-based markup language for describing the layout of a user interface in a JavaFX application.
- Classes extending <code>PluginView</code> and <code>PluginViewController</code> have to be implemented for testing whether the input is valid and for loading and saving data to and from XML.

All executors and process blocks integrated in Watchdog are using this plugin system. Hence, examples how to implement a new XML element can be found in the package de.lmu.ifi.bio.watchdog.xmlParser.plugins of the Java source code.

7 Docker

In order to run a Docker image, Docker must be installed and configured correctly as descibed <u>here</u>.

7.1 Install the Watchdog Docker image

A Watchdog image for Docker can be obtained from hub.docker.com. The image is rebuild automatically by the Bioconda project once a new version is released on Bioconda.

download the latest version You can of the image with docker pull klugem/watchdog-wms. Within the Docker image the environment variable WATCHDOG HOME is set automatically to the installation directory of Watchdog (required for the watchdogBase attribute). The -useEnvBase flag of the command line version can be used to override the watchdogBase attribute of the XML workflow with the value stored in WATCHDOG HOME. Moreover, the installation directory of Watchdog is mounted under /watchdog within the Docker image.

7.2 Sharing of files

In order to exchange files with the host system, the -v or -mount option of Docker can be used. These option can be used multiple times.

More information can be found in the <u>documentation</u> of Docker.

7.3 Port forwarding

In order to use the build-in webserver of Watchdog, the port used by the webserver must be forwarded to the host running the Docker container.

The command *docker run -p 8090:8080 image command* maps the container port 8080 (TCP) to the port 8090 (TCP) on the Docker host. More information can be found in the <u>documentation</u> of Docker.

7.4 How to use the Docker Watchdog image

The examples within the Docker image are automatically configured when {%Nwatchdog-cmd%N} is started the first time and are stored in /watchdog/examples. The command

```
docker run -h localhost -p 8080:8080 klugem/watchdog-wms watchdog-cmd -useEnvBase -x /watchdog/examples/example basic sleep.xml
```

executes the example described in <u>3.2</u> and forwards the webserver port to the host port 8080.

Alternatively, it is possible to run a workflow that is stored on the host system as described in <u>7.2</u>. Ensure that all files used in the workflow are made accessible within the Docker image.

7.5 Use Docker in modules

A Docker image can also be used in a module. The module <code>bowtie2Docker</code> implements an example module that uses the Docker image of <code>Bowtie 2</code> that is provided by <code>Bioconda</code> and hosted on <code>quay.io</code>. The Docker image will be automatically downloaded if it is not found locally.

Make sure that the Docker daemon is installed and running before you test this example.

Example 25: Example usage of the Bowtie 2 Docker module

```
<?xml version="1.0" encoding="UTF-8"?>
     <watchdog xmlns:xsi="http://www.w3.org/2001/XMLSchema-</pre>
instance" xsi:noNamespaceSchemaLocation="watchdog.xsd"
watchdogBase="{%INSTALL%}" isTemplate="true">
 4
          <settings>
 5
               <constants>
                    <const name="BASE">
{%INSTALL%}/modules/bowtie2Docker/example data</const>
               </constants>
 8
          </settings>
 9
          <tasks mail="{%MAIL%}">
10
               <bowtie2DockerTask id="1"</pre>
name="bowtie2 in docker">
12
                    <streams>
13
<stdout>/tmp/bowtie2.docker.test.out</stdout>
<stderr>/tmp/bowtie2.docker.test.err</stderr>
15
                    </streams>
16
                    <parameter>
<genome>${BASE}/index/lambda virus
18
                         <reads>${BASE}/reads/reads 1.fg</reads>
19
                         <reads>${BASE}/reads/reads 1.fq</reads>
20
<outfile>/tmp/bowtie2.docker.test.sam</outfile>
21
                    </parameter>
22
               </bowtie2DockerTask>
```

Example 25 shows how the <code>bowtie2Docker</code> module can be used with the provided example data. The test data that is shipped with Bowtie 2 is stored in the folder <code>example_data</code> of the module (6). Log files are written to <code>/tmp/bowtie2.docker.test.[out|err]</code> (13, 14) while the mapped reads are stored in SAM format in <code>/tmp/bowtie2.docker.test.sam</code> (20).