

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

New features in Watchdog 2.0:

- *[new]* execution: execute only altered or unfinished tasks (resume mode)
- *[new]* execution: detach from workflow execution and attach later on (detach/reattach mode)
- *[new]* execution: use custom before and after command scripts
- *[new]* execution: implementation of XML plugin supporting package managers and virtualizer
- *[new]* execution: support of Conda package manager for module dependencies
- *[new]* graphical user interface for module creation
- *[new]* documentation: standardized documentation format for modules
- *[new]* documentation: generation of module reference book
- *[new]* documentation: documentation template generator
- *[new]* reporting: module versioning
- *[new]* reporting: retrieval of third-party software versions
- *[new]* reporting: create report on workflow execution
- *[new]* sharing: [community_platform](#) for sharing of [modules](#) and [workflows](#)

2 Install and Configure Watchdog

2.1 Requirements

Watchdog is platform independent as it is written in Java. Hence, it requires JDK 11 or higher, which can be [obtained from Oracle](#) and installed on Windows, Linux, or macOS.

The GUI of the workflow designer and the *moduleMaker* depend on the JavaFX SDK 11 or higher. The JavaFX version obtained with the Maven build script is used by default, which is located in *jars/libs/modules/*.

Alternatively, it can be downloaded from [Gluon](#). An installation guide is provided [here](#). Both launcher bash scripts (*workflowDesigner.sh* and *moduleMaker.sh*) will try to identify the installation location of the JavaFX SDK automatically. If that fails or the installation location of the JavaFX SDK is known, the *JFX_SDK_LIB_PATH_ENV* environment variable can be used to set the path manually using *export JFX_SDK_LIB_PATH_ENV=/path/to/javafx/sdk/*.

Most Watchdog modules 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. After downloading, extract the provided archive into a folder of your choice (either using *tar xfvz watchdog.tar.gz* or *unzip watchdog.zip* depending on which archive you downloaded). 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 -c conda-forge watchdog-wms*. In that case the 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 [8](#).

Modules previously delivered with Watchdog are now located at the community github repository [watchdog-wms/watchdog-wms-modules](#). The reference book for all modules part of this repository is available at <https://watchdog-wms.github.io/watchdog-wms-modules>. Thus, as a next step you should download Watchdog modules from the [community github repository](#) and extract them into the *modules/* folder of the Watchdog directory. Alternatively, you can run *modules/downloadCommunityModules.sh* from the Watchdog directory.

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
- `documentation`: contains Watchdog's documentation in HTML- and PDF-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
- `jars`: runnable JAR-files that are build from Watchdog's source code
- `java_source`: Watchdog's source code
- `modules`: module folder that is used by default 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

The script `helper_scripts/dependencyTest.sh` can be used to test if software required by modules using a wrapper bash script is available via the `PATH` variable. For this purpose, software requirements have to be provided in the `$USED_TOOLS` variable of the bash script. In addition, availability of R and perl packages that are used in scripts are checked. During workflow execution availability of required software is also checked.

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, see 2.5 for E-mail server configuration)
```

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 JAR Files

These runnable JAR-files (except `moduleMaker.jar`) are shipped together with Watchdog in the `jars/` subdirectory of the Watchdog installation folder.

- `watchdog.jar`: command-line tool that executes Watchdog workflows

- *watchdogDesigner.jar*: graphical user interface for workflow design and execution
- *moduleMaker.jar*: provides a graphical user interface for module creation
- *docuTemplateExtractor.jar*: generates templates for module documentation
- *refBookGenerator.jar*: creates a module reference book based on a set of modules
- *reportGenerator.jar*: basic reporting of steps performed during execution of a workflow
- *moduleValidator.jar*: command-line tool that can be used to verify integrity of modules
- *workflowValidator.jar*: command-line tool that can be used to verify integrity of workflows
- *watchdog-[DEV|RELEASE].jar*: contains the compiled Watchdog classes, which are invoked by all other JARs

More information on how to use these programmes can be found in the manual in section [6](#). Please note that the *moduleMaker* is not shipped with Watchdog but can be obtained by running *helper_scripts/downloadModuleMaker.sh* located in the Watchdog installation directory. See [watchdog-wms/moduleMaker](#) for more information.

2.4 Getting started

Once Watchdog is correctly installed, you can run example workflows shipped with Watchdog. To configure them run *helper_scripts/configureExamples.sh -i /path/to/install/folder/of/watchdog [-m your@mail-address.com]*. Afterwards, the example workflows are located in *examples/* and can be started using *./watchdog.sh -x path2/xml-file.xml*.

- *example_basic_sleep.xml* - basic example with one task to show XML workflow structure
- *example_dependencies.xml* - workflow with dependencies between tasks
- *example_execution_environments.xml* - workflow using different execution environments (requires modifications)
- *example_process_blocks.xml* - shows how to work with process sequences, folders and tables
- *example_execution_wrapper.xml* - module dependencies are obtained by the Conda package manager (requires modifications)
- *example_task_actions.xml* - introduces task actions using the example of a file copy action
- *example_checkers.xml* - shows how to use a custom success checker
- *example_docker.xml* - uses a module that internally uses a docker image containing bowtie2
- *example_include.xml* - shows how to use additional module folders
- *example_simple_calculations.xml* - usage of simple mathematical calculations within a workflow
- *example_constant_replacement.xml* - shows to to use constants in workflows
- *example_environment_variables.xml* - setting environment variables

- `example_mail_notification.xml` - example with mail notifications on completed subtasks and checkpoints
- `example_streams.xml` - redirection of stdout and stderr streams
- `workflow1_basic_information_extraction.xml` - simple workflow that extracts information from files using basic UNIX tools
- `workflow2_differential_gene_expression.xml` - workflow performing a differential gene expression analysis on an example data set (needs bwa and ContextMap2 to be installed and configured)

More information on these example workflows can be found in section [3](#) and [4](#).

An introduction on how to use the workflow designer (GUI) can be found [here](#).

2.5 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 will 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 `-mailConfig` 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

```
1 mail.smtp.auth true
2 mail.smtp.host smtp.googlemail.com
3 mail.smtp.port 587
4 mail.smtp.user johns_watchdog@gmail.com
5 mail.smtp.pw r9x741(klsab
6 mail.smtp.from johns_watchdog@gmail.com
7 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.

2.6 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 authentication can be generated using the tool *ssh-keygen* that is part of *openssh*. If you need further information you can find many online tutorials that explain how to use a private key for ssh authentication. E.g. [How To Set Up SSH Keys](#) and [SSH/OpenSSH/Keys](#)

2.7 DRMAA 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:
 1. 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.

Alternatively, binary-based executors can be used, which are currently implemented for SLURM and SGE. The required control binaries must be accessible via the *\$PATH* variable.

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

```
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="sleepTaskParameterType">
6          <x:all>
7              <x:element name="wait" type="paramWait_sleep"
minOccurs="1" maxOccurs="1" />
8          </x:all>
9      </x:complexType>
10
11      ...
12
13      <!-- make task definition available via substitution
group -->
14      <x:element name="sleepTask" type="sleepTaskType"
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($value,
'($[A-Za-z_]+)|($(.+))|([({}($[A-Za-z_]+(,s*){0,1}){0,1}([0-
9]+(,s*){0,1}){0,1}[]))') or matches($value, '^([0-9]+[smhd]
{0,1}$)'" 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 *sleepTaskParameterType* (5-9). In this case only one parameter named *wait* 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 *matches()* 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 *name* 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 *sleepTask*.

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 address 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

```
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>
10                     <wait>30s</wait>
11                 </parameter>
12             </sleepTask>
```

```

13         </tasks>
14     </watchdog>

```

Example 3 shows a most basic XML file that contains only a single task named *sleep*. Every XML file that should be parsed by Watchdog must contain a `<watchdog>` element as root element (2). The attribute `watchdogBase` of it must refer to the folder in which Watchdog was installed. The attribute `isTemplate` 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 `<tasks>` the tasks which should be executed must be defined (5). Each task must contain an `id` and `name` attribute (8). With the `<parameter>` 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 `<flagName>true</flagName>` or `<flagName>1</flagName>` while parameters can be set with `<paramName>value</paramName>` (10).

Table 1: Attributes in the context of Watchdog

element	attribute	type	function
<code><watchdog></code>	<code>watchdogBase</code>	string	path to the install path of watchdog
<code><watchdog></code>	<code>isTemplate</code>	boolean	prevents Watchdog from executing unconfigured workflow templates; default: <i>false</i>
<code><tasks></code>	<code>[mail]</code>	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
<code><tasks></code>	<code>[projectName]</code>	string	name of the complete process; default: not set
<code><?Task></code>	<code>[id]</code>	integer	numeric id of the task; if not set all id's will be automatically generated; default: not set
<code><?Task></code>	<code>name</code>	string	name of the task
<code><?Task></code>	<code>[processBlock]</code>	string	processBlock as source of varying parameters (see 4.1)
<code><?Task></code>	<code>[executor]</code>	string	execution environment on which the task is executed (see 4.3)
<code><?Task></code>	<code>[environment]</code>	string	use globally defined environment variables (see 4.6)
<code><?Task></code>	<code>[maxRunning]</code>	integer	maximal number of simultaneously running tasks; default: not restricted
<code><?Task></code>	<code>[notify]</code>	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: <i>disabled</i> (see 4.7)
<code><?Task></code>	<code>[checkpoint]</code>	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; default: <i>disabled</i>
<code><?Task></code>	<code>[confirmParam]</code>	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: <i>disabled</i>
<code><?Task></code>	<code>[version]</code>	integer	version of the module that should be used for that task; default: <i>1</i> (see 5.6)
<code><?Task></code>	<code>[posX]</code>	integer	x coordinate for display in GUI; default: not set
<code><?Task></code>	<code>[posY]</code>	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:

- `<processBlock>` - process a task with varying parameters (see [4.1](#))
- `<executors>` - define different executor environments (see [4.3](#))
- `<wrappers>` - execution wrappers usable as package managers or for virtualization (see [4.4](#))
- `<constants>` - defines constants that substitute placeholders (see [4.5](#))
- `<environments>` - define or update environment variables (see [4.6](#))
- `<modules>` - define multiple module include directories (see [4.11](#))

Apart from the `<parameter>` element, the following elements are allowed in `<?Task>` elements:

- `<environment>` - define or update environment variables (see [4.6](#))
- `<dependencies>` - define dependencies between tasks (see [4.2](#))
- `<streams>` - define location of standard streams and set a working directory (see [4.8](#))
- `<checkers>` - usage of custom success or error checkers (see [4.12](#))
- `<actions>` - define task actions that are performed before or after tasks execution (see [4.9](#))

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
- `<processFolder>` - argument is a path to a file
- `<processInput>` - multiple arguments obtained from dependencies
- `<processTable>` - multiple arguments stored in a tab-separated file with names of variables stored in the first line

When the `<processBlock>` attribute of a task is set the argument of the process folder or sequence is substituted at run time within `<parameter>`, `<streams>`, `<checkers>`, `<actions>` and `<environment>` elements in the following manner:

- `<processSequence>` - `[]/{}/()` -> number
- `<processFolder>` - `{}` -> absolute path to the file
- `<processFolder>` - `()` -> absolute path to the parent folder of the file
- `<processFolder>` - `[]` -> name of the file

- **<processFolder>** - [*n*]/[*n*] -> *n* suffixes of the filename are truncated using . as separator
- **<processFolder>** - (*n*) -> *n* suffixes of the parent folder are truncated using / as separator
- **<processFolder>** - ([*n,sep*]) -> suffixes of the value are truncated using *sep* as separator (might also be a regex)
- **<processTable>** - ([*\$COL_NAME*]) -> value stored in the column named *\$COL_NAME*
- **<processTable>** - ([*\$COL_NAME,n,sep*]) -> value stored in the column named *\$COL_NAME* but with suffix truncation as described above
- **<processInput>** - ([*\$RET_NAME*]) -> return value of a dependency with the name *\$RET_NAME*
- **<processInput>** - ([*\$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

```

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      <settings>
5          <!-- definition of different process blocks -->
6          <processBlock>
7              <processSequence name="qualities" start="1"
end="9" step="2" />
8              <processFolder name="specialFiles" folder="
{%EXAMPLE_DATA%}/spec/" pattern="*.spec" />
9              <baseFolder folder="{%EXAMPLE_DATA%}/">
10                 <processFolder name="txtFiles"
folder="txt/" pattern="*.txt" />
11                 <processFolder name="txtFiles"
folder="other_txt/" pattern="*.txt" append="true" maxDepth="1" />
12                 <processFolder name="gzFiles"
folder="txt_zipped/" pattern="*.gz" disableExistenceCheck="true"
/>
13                 <processTable name="sleepTable"
table="processTable.input.txt" />
14             </baseFolder>
15         </processBlock>
16     </settings>
17
18     <tasks mail="{%MAIL%}">
19         <!-- compress all files with *.txt ending in

```

```

/some/base/folder/TXT -->
20         <gzipTask id="1" name="compress files"
processBlock="txtFiles" checkpoint="enabled">
21             <parameter>
22                 <input>{}</input>
23                 <output>
24                 {%EXAMPLE_DATA%}/txt_zipped/[1].gz</output>
25             </parameter>
26         </gzipTask>
27
28         <!-- test quality values 1,3,5,7 and 9 -->
29         <gzipTask id="2" name="quality test"
processBlock="qualities" checkpoint="subtask">
30             <dependencies>
31                 <depends>1</depends>
32             </dependencies>
33             <parameter>
34                 <input>
35                 {%EXAMPLE_DATA%}/txt/txtFile1.txt</input>
36                 <output>
37                 {%EXAMPLE_DATA%}/qualityTest/txtFile1_q[].gz</output>
38                 <quality>[]</quality>
39             </parameter>
40             <environment>
41                 <var name="QUALITY">{}</var>
42             </environment>
43         </gzipTask>
44
45         <!-- sleep tasks which are created based on a
process table -->
46         <sleepTask id="3" name="table sleep"
processBlock="sleepTable">
47             <dependencies>
48                 <depends>2</depends>
49             </dependencies>
50             <streams>
51                 <stdout>{$OUT, 1}</stdout>
52             </streams>
53             <parameter>
54                 <wait>{$DURATION}</wait>
55             </parameter>
56             <environment>
57                 <var name="IMPORTANT_ID_RAW">
58                 [$IMPORTANT_ID]</var>
59                 <var
name="IMPORTANT_ID_CALC">$( [$IMPORTANT_ID] *3)</var>
60             </environment>
61         </sleepTask>
62     </tasks>
63 </watchdog>

```


Example 4 shows three different ways how process blocks can be specified. First a `<processSequence>` named `qualities` is defined that creates the numbers 1,3,5,7 and 9 (7). In the next line a `<processFolder>` 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 `<processFolder>` is a child element of a `<baseFolder>`, the `folder` attribute of the `<processFolder>` will be prefixed with the `folder` attribute of the `<baseFolder>` (9-14). The attribute `disableExistenceCheck` that is enabled for the `<processFolder>` with the name `gzFiles` causes Watchdog not to force the existence of the folder when it is started (12).

The task with `id 1` will compress all `.txt` files in the folders `{%EXAMPLE_DATA%}/txt` and `{%EXAMPLE_DATA%}/other_txt` and store them in `{%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 `txtFile1_q` as prefix and the used quality as suffix in `{%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 columns of a `<processTable>` 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 [4.10](#) (55).

Table 2: Attributes in the context of process blocks

element	attribute	type	function
<code><?ProcessBlock></code>	<code>name</code>	string	is used as reference in the <code>processBlock</code> attribute of a task
<code><?Task></code>	<code>processBlock</code>	string	name of a <code><?ProcessBlock></code> element
<code><?ProcessBlock></code>	<code>[append]</code>	boolean	if set to true, two or more process blocks of the same type can be merged; supported by processSequence and ProcessFolder; default: <code>false</code>
<code><processSequence></code>	<code>start</code>	double	inclusive start of the numeric series
<code><processSequence></code>	<code>[step]</code>	double	number that is added until the value is greater than end; default: <code>1</code>
<code><processSequence></code>	<code>end</code>	double	break condition, might be inclusive
<code><processFolder></code>	<code>folder</code>	integer	absolute or relative to a <code><baseFolder></code> path to a folder
<code><processFolder></code>	<code>pattern</code>	string	pattern selecting files that should be substituted; syntax as in bash
<code><processFolder></code>	<code>[ignore]</code>	string	files matching that pattern will be ignored; syntax as in bash; default: not set
<code><processFolder></code>	<code>[disableExistenceCheck]</code>	boolean	folder must not exist when Watchdog is started; default: <code>false</code>
<code><processFolder></code>	<code>[maxDepth]</code>	integer	a positive integer will cause that <code>maxDepth</code> levels of subdirectories are traversed while by default only the parent folder is processed; default: <code>0</code>
<code><baseFolder></code>	<code>folder</code>	string	absolute path which is used as prefix before the path of the <code><processFolder></code> is added
<code><baseFolder></code>	<code>[maxDepth]</code>	integer	see description of <code><processFolder></code> <code>[maxDepth]</code> ; if both are set, the value of the <code><processFolder></code> element is set; default: <code>0</code>
<code><processTable></code>	<code>table</code>	string	path to a tab-separated file with header; the column names must consist out of [A-Za-z_]
<code><processTable></code>	<code>[disableExistenceCheck]</code>	boolean	table file must not exist when Watchdog is started; default: <code>false</code>

element	attribute	type	function
<processTable>	[compareName]	column	name that should be used to compare names of separate dependencies; default: complete line
<processInput>	sep	string	separator which is used to join multiple values of global dependencies together; default: .
<processInput>	[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

```

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      <settings>
5          <!-- definition of two process folders -->
6          <processBlock>
7              <baseFolder folder="{%EXAMPLE_DATA%}/">
8                  <processFolder name="txtFiles"
folder="txt/" pattern="*.txt" />
9                  <processFolder name="gzFiles"
folder="txt_zipped/" pattern="*.gz" disableExistenceCheck="true"
/>
10                 </baseFolder>
11             </processBlock>
12         </settings>
13
14         <tasks mail="{%MAIL%}">
15             <!-- definition a simple sleep task -->
16             <sleepTask id="1" name="sleep">
17                 <parameter>
18                     <wait>30s</wait>
19                 </parameter>
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>
27                 {%EXAMPLE_DATA%}/txt_zipped/[1].gz</output>
28             </parameter>
29             <!-- dependency definition -->
30             <dependencies>
31                 <depends>1</depends>
32             </dependencies>
33         </gzipTask>
34         <!-- decompress all files with *.gz ending in
/some/base/folder/TXT_ZIPPED -->
35         <gzipTask id="3" name="decompress"
processBlock="gzFiles">
36             <parameter>
37                 <input>{}</input>
38                 <output>
39                 {%EXAMPLE_DATA%}/txt_decompressed/[1].txt</output>
40                 <decompress>true</decompress>
41             </parameter>
42             <!-- dependency definition -->
43             <dependencies>
44                 <depends separate="true" prefixName="
[1]">2</depends>
45             </dependencies>
46         </gzipTask>
47     </tasks>
</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>			parent of <depends> elements and child of <?Task>
<depends>		integer	already defined task id on which the task should depend on
<depends>	[separate]	boolean	if set to <i>true</i> each subtask depends only on its corresponding subtask; default: <i>false</i>
<depends>	[keep4Slave]	boolean	if set to <i>true</i> 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: <i>false</i>

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

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 using DRMAA
- `<sge>` - task is executed on a SGE computer cluster using control binaries
- `<slurm>` - task is executed on a SLURM computer cluster using control binaries

Example 6: Definition of different execution environments

```

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      <settings>
5          <!-- examples of different execution environments
-->
6          <executors>
7              <local name="localhost" maxRunning="2" />
8              <sge name="defaultCluster" default="true"
memory="1G" beforeScripts="ulimitMemory.sh" queue="short.q" />
9              <sge name="highPerformanceCluster" slots="4"
memory="3G" maxRunning="4" queue="short.q" />
10             <remote name="superComputer"
user="mustermann" host="superComputer"
privateKey="/path/to/private/auth/key" port="22"
disableStrictHostCheck="false" />
11         </executors>
12     </settings>
13
14     <tasks mail="{%MAIL%}">
15         <!-- execute this task on the localhost -->
16         <sleepTask id="1" name="sleep"
executor="localhost">
17             <parameter>
18                 <wait>30s</wait>

```

```

19             </parameter>
20         </sleepTask>
21     </tasks>
22 </watchdog>

```

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). Before the actual module command is executed on that executor, the commands stored in the before script *ulimitMemory.sh* are executed. If a relative path is given, the script must be located in *core_lib/executor_scripts*. In this example the script will enforce that the requested memory is not exceeded using the *ulimit* command.

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 [2.6](#) and [2.7](#)).

Table 4: Attributes in the context of execution environments

element	attribute	type	function
<?Executor>	name	string	is used as reference in the executor attribute of a task
<?Task>	executor	string	name of a <?Executor> element
<?Executor>	[environment]	string	environment with that name is used as default environment; default: not set
<?Executor>	[default]	boolean	defines which execution environment is taken as default; default: <i>false</i>
<?Executor>	[maxRunning]	integer	number of tasks that can run at the same time; default: not restricted
<?Executor>	[workingDir]	string	working directory to which the executor switches before task execution; default: <i>/usr/local/storage/</i>
<?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: <i>false</i>
<?Executor>	[maxSlaveRunning]	integer	number of tasks that can run at the same time on a slave if stickToHost is enabled; default: 1

element	attribute	type	function
<code><? Executor></code>	<code>[pathToJava]</code>	string	path to java binary which is used for slave mode execution; default: <code>/usr/bin/java</code>
<code><? Executor></code>	<code>[shebang]</code>	string	shebang, which is used if a temporary script is build that defines environment variables or before/after script commands; default: <code>#!/bin/bash</code>
<code><? Executor></code>	<code>[beforeScripts]</code>	string	path to a script containing commands that are executed before the actual module command; multiple scripts can be provided by using ':' as separator; default: not set
<code><? Executor></code>	<code>[afterScripts]</code>	string	path to a script containing commands that are executed after the actual module command; multiple scripts can be provided by using ':' as separator; default: not set
<code><? Executor></code>	<code>packageManagers</code>	string	list of name(s) of <code><?Wrapper></code> package manager separated by ','
<code><? Executor></code>	<code>container</code>	string	name of a <code><?Wrapper></code> virtualizer
<code><remote></code>	<code>user</code>	string	name of the user on the remote host system
<code><remote></code>	<code>host</code>	string	name of the host which should be used for execution; multiple hostnames must be separated by ';' - in that case the <code>maxRunning</code> argument is applied on each host separately
<code><remote></code>	<code>privateKey</code>	string	path the to private ssh auth key; should be protected by a passphrase!
<code><remote></code>	<code>[port]</code>	integer	port which is used for the ssh connection; default: <code>22</code>
<code><remote></code>	<code>[disableStrictHostCheck]</code>	boolean	disables the validation of the public key of the host; not recommended!; default: <code>false</code>
<code><cluster></code>	<code>[customParameters]</code>	string	additional parameters that are directly passed to the DRMAA system without further processing; default: not set
<code><sge></code>	<code>[slots]</code>	integer	number of cores which are reserved on the computer cluster; default: <code>1</code>
<code><sge></code>	<code>[memory]</code>	string	memory per slot suffixed with M (megabyte) or G (gigabyte); default: <code>3000M</code>
<code><sge></code>	<code>[queue]</code>	string	queue on which the tasks should run on the computer cluster; default: not set
<code><sge></code>	<code>[disableDefault]</code>	boolean	default parameters are ignored; default: <code>false</code>
<code><sge></code>	<code>[customParameters]</code>	string	additional parameters that are directly passed to the SGE system without further processing; default: not set
<code><slurm></code>	<code>cluster</code>	string	cluster to communicate with; default: not set
<code><slurm></code>	<code>[cpu]</code>	integer	number of cores which are reserved on the computer cluster; default: <code>1</code>
<code><slurm></code>	<code>[memory]</code>	string	memory per slot suffixed with M (megabyte) or G (gigabyte); default: <code>3000M</code>
<code><slurm></code>	<code>[partition]</code>	string	partition of the cluster on which the job should be executed; default: not set
<code><slurm></code>	<code>[timelimit]</code>	string	maximum time the task will require to complete; default: <code>0-12:0</code>
<code><slurm></code>	<code>[disableDefault]</code>	boolean	default parameters are ignored; default: <code>false</code>
<code><slurm></code>	<code>[customParameters]</code>	string	additional parameters that are directly passed to the SLURM system without further processing; default: not set

4.4 Execution wrappers

Execution wrappers can be used in combination with `<?Executor>` as package managers or virtualizer. Multiple execution wrappers can be defined within the `<wrappers>` element.

Implemented package managers:

- **<conda>** - tasks are executed in a Conda environment if supported by the module

Implemented virtualizer:

- **<docker>** - WIP

Example 7: Definition of Conda execution wrapper

```
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      <settings>
4          <!-- definition of execution wrappers -->
5          <wrappers>
6              <!-- TODO: modify path2conda and
path2environments-->
7              <conda name="condaWrapper"
path2conda="/your/path/to/conda/"
path2environments="/tmp/conda_watchdog_env/" />
8          </wrappers>
9          <!-- local executor that will use the package
manager condaWrapper for supporting modules -->
10         <executors>
11             <local name="localhost"
packageManagers="condaWrapper" />
12         </executors>
13     </settings>
14     <tasks>
15         <!-- definition of a simple sleep task, which will
be executed in a Conda environment -->
16         <sleepTask id="1" name="sleep"
executor="localhost">
17             <parameter>
18                 <wait>10s</wait>
19             </parameter>
20         </sleepTask>
21     </tasks>
22 </watchdog>
```

In example 7 a Conda execution wrapper is defined as child of the **<wrappers>** element (5-8). The wrapper will be used for tasks that were created from modules that support the Conda package manager wrapper (7). The attribute **path2conda** defines the Conda installation to use. Conda environments are initialized once per module and stored in the **path2environments** directory.

In line 11, a localhost executor is defined that uses the previously defined execution wrapper named *condaWrapper*.

Table 5: Attributes in the context of execution wrappers

element	attribute	type	function
<?Wrapper>	name	string	is used as reference in the packageManagers or container attribute of an executor
<?Executor>	packageManagers	string	list of name(s) of <?Wrapper> package manager separated by ','
<?Executor>	container	string	name of a <?Wrapper> virtualizer
<conda>	path2conda	string	absolute path to Conda installation directory
<conda>	[path2environments]	string	path to directory in which Conda environments will be installed; path can also be relative to path2conda; default: conda_watchdog_env/

4.5 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 are two pre-defined constants. The first is named *\${TMP}* and is substituted within **<?Task>** tags with the working directory of the executor that will execute the task. The second is named *\${WF_PARENT}* and is replaced with the parent folder containing the XML workflow file.

Example 8: Definition and use of global constants

```

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      <settings>
5          <!-- definition of a constant named WAIT_TIME -->
6          <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
13     <tasks mail="{%MAIL%}">
14 
```

```

15         <!-- definition a simple sleep task with constant
replacement -->
16         <sleepTask id="1" name="sleep test">
17             <streams>
18
19 <stdout>${LOG_BASE}/${FILE_NAME}.out</stdout>
19             </streams>
20             <parameter>
21                 <wait>${WAIT_TIME}</wait>
22             </parameter>
23         </sleepTask>
24     </tasks>
25 </watchdog>

```

In example 8 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 6: Attributes in the context of global constants

element	attribute	type	function
<code><constants></code>			parent of <code><const></code> elements and child of <code><settings></code>
<code><const></code>	<code>name</code>	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
<code><const></code>		string	replacement value

4.6 Environment variables

Some tools expect specific environment variables to be set correctly. For example the **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 9: Definition of environment variables

```
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      <settings>
5          <!-- definition of a environment -->
6          <environments>
7              <environment name="pathEnv">
8                  <var name="PATH"
update="true">~/software/bin</var>
9                  </environment>
10             </environments>
11         </settings>
12
13         <!-- begin task block and use that mail to inform the
user on success or failure -->
14         <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"
sep="@">separator test</var>
26                 </environment>
27             </envTask>
28         </tasks>
29     </watchdog>
```

In example 9 an environment named *pathEnv* is defined in which the variable *PATH* is updated (8). The entry *~/software/bin* is added at the beginning of the *PATH* variable and after the default separator character the previous value is kept. The *environment* attribute of the *env* 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 */bin/sh* while the second one updates a variable called *TEST* using an alternative separator.

Table 7: Attributes in the context of environment variables

element	attribute	type	function
<environment>	name	string	is used as reference in the <code>environment</code> attribute of a task
<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: <code>false</code>
<environment>	[useExternalExport]	boolean	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: <code>true</code>
<environment>	[exportCommand]	string	custom command to set a environment variable; <code>{ \$NAME }</code> and <code>{ \$VALUE }</code> are substituted and must be part of the command; default: <code>export { \$NAME }="{ \$VALUE }"</code>
<?Task>	environment	string	name of a <environment> element
<var>		string	value of the environment variable
<var>	name	string	name of the environment variable
<var>	[update]	boolean	if <code>true</code> the value is added at the beginning of the variable and the old values comes afterwards separated with the value stored in the <code>sep</code> attribute; default: <code>false</code>
<var>	[sep]	string	separator which is used when the value of the variable should be updated; default: <code>:</code>
<var>	[copyLocalValue]	boolean	copies the environment variables with the name <code>name</code> which is set on the host running Watchdog; default: <code>false</code>

4.7 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 10: Different mail notification options

```

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      <settings>
5          <!-- definition of different process blocks -->
6          <processBlock>
7              <processSequence name="sleepTime" start="5"
end="15" step="5" />
8          </processBlock>
9      </settings>
10
11     <!-- 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 -->
14         <sleepTask id="1" name="sleep simple"
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"
22     notify="subtask" processBlock="sleepTime">
23         <parameter>
24             <wait>[]s</wait>
25         </parameter>
26     </sleepTask>
27 </tasks>
</watchdog>

```

In example 10 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 8: Attributes in the context of mail notification

element	attribute	type	function
<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

4.8 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 occur in the same order as they are listed in the following: **<workingDir>**, **<stdout>**, **<stderr>** and **<stdin>** (but each of them is optional)

Example 11: 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>
10                 <wait>30s</wait>
11             </parameter>
12             <!-- definition of a standard output location
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 11 the working directory is set to `/tmp` (14). Afterwards, the standard output of the `sleep` task is written to the file `{%EXAMPLE_DATA%}/sleepTest.out` (15). The standard error stream is appended at the end of a file named `/tmp/sleepTest.err` (16).

Table 9: Attributes in the context of standard streams_and_working_directory

element	attribute	type	function
<code><streams></code>		boolean	saves used resources to .res if standard output stream is saved to a file; default: <code>false</code>
<code><workingDir></code>		string	sets a custom working directory before the tool is executed; default: <code>/usr/local/storage</code>
<code><stdout></code>		string	writes standard output stream into file; default not saved
<code><stderr></code>		string	writes standard error stream into file; default not saved
<code><stdin></code>		string	file is used as standard input; default: not set
<code><stdin></code>	<code>[disableExistenceCheck]</code>	boolean	file must not exist when Watchdog is started; default: <code>false</code>
<code><stdout>/<stderr></code>	<code>[append]</code>	boolean	appends the stream at the end of the file; default: <code>false</code>

4.9 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 especially 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 found [here](#). However, any file system with an implementation of the *FileProvider* can also be included by the user as described in [7.1](#).

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 12: Definition of task actions

```
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      <tasks mail="{%MAIL%}">
5          <gzipTask id="1" name="gzip task">
6              <parameter>
7                  <!-- path to a file that does not exist
yet -->
8
<input>/tmp/watchdog_file_to_compress.tmp</input>
9                  </parameter>
10                 <!-- action that copies a to the input
location -->
11                 <actions time="beforeTask">
12                     <copyFile file="
{%INSTALL%}examples/example_task_actions.xml"
```

```

destination="/tmp/watchdog_file_to_compress.tmp" override="true"
/>
13             </actions>
14         </gzipTask>
15     </tasks>
16 </watchdog>

```

In example 12 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).

Table 10: Attributes in the context of actions

element	attribute	type	function
<code><actions></code>	<code>time</code>	enum	defines when the task action block is executed; <code>beforeTask</code> : before the task is executed; <code>afterTask</code> : after the task is executed; <code>onSuccess</code> : when the task was successfully executed; <code>onFailure</code> : when task execution failed; <code>beforeTerminate</code> : before Watchdog or a slave terminates itself
<code><actions></code>	<code>[uncoupleFromExecutor]</code>	boolean	if enabled, task actions are executed on the host running Watchdog instead of the execution host; default: <code>false</code>
<code><createFile></code>	<code>file</code>	string	path to the file that should be created
<code><createFile></code>	<code>[override]</code>	boolean	defines if an existing file should be overwritten; default: <code>false</code>
<code><createFile></code>	<code>[createParent]</code>	boolean	defines if the parent directories should be created if nonexistent; default: <code>true</code>
<code><createFolder></code>	<code>folder</code>	string	path to the folder that should be created and will be empty if action succeeds
<code><createFolder></code>	<code>[override]</code>	boolean	defines if an existing folder should be deleted; default: <code>false</code>
<code><createFolder></code>	<code>[createParent]</code>	boolean	defines if the parent directories should be created if nonexistent; default: <code>true</code>
<code><copyFile></code>	<code>file</code>	string	path to the file that should be copied
<code><copyFile></code>	<code>destination</code>	string	path to the destination of the new file
<code><copyFile></code>	<code>[override]</code>	boolean	defines if an existing file should be overwritten; default: <code>false</code>
<code><copyFile></code>	<code>[deleteSource]</code>	boolean	deletes the source file after the copy operation; default: <code>false</code>
<code><copyFile></code>	<code>[createParent]</code>	boolean	defines if the parent directories should be created if nonexistent; default: <code>true</code>
<code><copyFolder></code>	<code>folder</code>	string	path to the folder that should be copied
<code><copyFolder></code>	<code>destination</code>	string	path to the destination folder
<code><copyFolder></code>	<code>[pattern]</code>	string	pattern selecting files that should be copied in that folder; syntax as in bash
<code><copyFolder></code>	<code>[override]</code>	boolean	defines if an existing folder should be deleted; default: <code>false</code>
<code><copyFolder></code>	<code>[deleteSource]</code>	boolean	deletes the source folder after the copy operation; default: <code>false</code>
<code><copyFolder></code>	<code>[createParent]</code>	boolean	defines if the parent directories should be created if nonexistent; default: <code>true</code>
<code><deleteFile></code>	<code>file</code>	string	path to the file that should be deleted

element	attribute	type	function
<code><deleteFolder></code>	<code>folder</code>	string	path to the folder that should be deleted
<code><deleteFolder></code>	<code>[pattern]</code>	string	pattern selecting files that should be deleted in that folder; syntax as in bash

4.10 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`. Additionally 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 13: Definition of simple calculations

```

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      <settings>
5          <!-- definition of two process blocks -->
6          <processBlock>
7              <processSequence name="sleepTime" start="1"
end="5" step="1.5" />
8              <processFolder name="txtFiles" folder="
{%EXAMPLE_DATA%}/txt/" pattern="*.txt" />
9          </processBlock>
10         </settings>
11
12         <tasks mail="{%MAIL%}">
13             <!-- sleep task with a simple calculation -->
14             <sleepTask id="1" name="sleep"
processBlock="sleepTime">
15                 <parameter>
16                     <wait>$( (i+1)^2-1)s</wait>
17                 </parameter>
18             </sleepTask>
19
20             <!-- compress txt files and write log files to
()/log/* -->
21             <gzipTask id="2" name="quality test"
processBlock="txtFiles">
22                 <streams>
23                     <stdout>()/log/$(x).out</stdout>
24                 </streams>
25                 <parameter>
26                     <input>{}</input>

```

```

27             <output>{}.gz</output>
28             <quality>3</quality>
29         </parameter>
30     </gzipTask>
31 </tasks>
32 </watchdog>

```

In example 13 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).

4.11 Multiple module search folders

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

Example 14: Definition of multiple module include folders

```

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      <settings>
5          <!-- TODO: modify one of these folders
{%INSTALL%}myCustomFolder/ or -->
6          <!-- /home/TODO/additionalModules/ to match a
folder that contains the 'sleep' module -->
7          <modules defaultFolder="myCustomFolder/">
8
<folder>/home/TODO/additionalModules/</folder>
9          </modules>
10     </settings>
11
12     <!-- begin task block and use that mail to inform the
user on success or failure -->
13     <tasks mail="{%MAIL%}">
14         <!-- definition a simple sleep task -->
15         <sleepTask id="1" name="sleep">
16             <parameter>
17                 <wait>30s</wait>
18             </parameter>
19         </sleepTask>
20     </tasks>
21 </watchdog>

```


In example 14 the default directory is changed to *myCustomFolder/* with the **defaultFolder** 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 *{%INSTALL%}/myCustomFolder/* and */home/additionalModules/*. In order to test that example you must create a new folder, copy the *sleep* module from Watchdog's module folder and adapt the path in line 7 or 8 to match that folder.

Table 11: Attributes in the context of module include_folders

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

4.12 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.Imu.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 15: Load custom checkers

```

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>
10                     <wait>30s</wait>
11                 </parameter>

```



```

12             <checkers>
13                 <!-- load a success checker with one
additional constructor argument -->
14                 <!-- it will check, if the file
{%INSTALL%}examples/mail_config exists and is not empty -->
15                 <checker classPath="
{%EXAMPLE_DATA%}/OutputFileExistsSuccessChecker.class"
className="de.lmu.ifi.bio.watchdog.successChecker.OutputFileExistsS
type="success">
16                     <cArg type="string">
{%INSTALL%}examples/mail_config</cArg>
17                 </checker>
18             </checkers>
19         </sleepTask>
20     </tasks>
21 </watchdog>

```

Example 15 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 12: Attributes in the context of custom checkers

element	attribute	type	function
<checker>	type	enum	type of the checker; success: checker should be used as success checker; error: checker is used as error checker
<checker>	className	string	complete class name including the package the class is located in
<checker>	classPath	string	absolute path to the compiled java class file
<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 16. 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.

Alternatively, the newly developed GUI `moduleMaker` (available at watchdog-wms/moduleMaker) can be used to automatically extract parameters and flags from a software help page to more conveniently create the corresponding module. See [2.3](#) for installation hints.

Example 16: Basic XSD structure

```
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  ...
5
6  </x:schema>
```

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

5.1 Input parameter definition

Example 17 shows how input parameters and flags can be defined.

Example 17: Input parameter

```
1  <!-- definition of the task parameters -->
2  <x:complexType name="nameOfModuleTaskParameterType">
3      <x:all>
4          <x:element name="parameter1"
type="paramAbsolutePath" minOccurs="1" maxOccurs="1" />
5          <x:element name="parameter2" type="paramString"
minOccurs="0" maxOccurs="unbounded" />
6          <x:element name="flag1" type="paramBoolean"
minOccurs="0" maxOccurs="1" />
```

```

7         </x:all>
8     </x:complexType>

```

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 18.

Example 18: Input parameter

```

1  <!-- module specific parameter types -->
2  <x:complexType name="paramWait_sleep">
3      <x:simpleContent>
4          <x:restriction base="paramString">
5              <x:assertion test="matches($value, '(${[A-Za-
z_]+})|($(.+))|([([({[A-Za-z_]+(,s*){0,1}}{0,1}([0-9]+(,S*)
{0,1}}{0,1}[[]]))])' ) or matches($value, '^([0-9]+[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 [5.3](#).

Example 19: Output parameter

```

1  <!-- define output parameters which must be written to a
file -->
2  <x:complexType name="nameOfModuleTaskReturnType">

```

```

3         <x:complexContent>
4             <x:extension base="taskReturnType">
5                 <x:all>
6                     <x:element name="outputParam1"
type="x:string" />
7                 </x:all>
8             </x:extension>
9         </x:complexContent>
10    </x:complexType>

```

Line 6 in example 19 specifies that the module must return a parameter named *outputParam1* of type *x:string*. 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 *writeParam2File* and *blockUntilFileIsWritten* defined in *core_lib/functions.sh* can be used.

5.3 Binary call command and other settings

Now the command that will be executed can be defined. Example 20 specifies that a script named *nameOfModule.sh* that is stored in *modules/nameOfModule* will be called.

Example 20: Binary call command

```

1    <!-- set command and other settings -->
2    <x:complexType name="nameOfModuleTaskOverrideType">
3        <x:complexContent>
4            <x:restriction base="baseAttributeTaskType">
5                <x:attribute name="binName" type="x:string"
fixed="nameOfModule.sh" />
6            </x:restriction>
7        </x:complexContent>
8    </x:complexType>

```

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 passing 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: *,*
- *versionQueryParameter*: parameter of the *binName* command used to query software versions of third-party software; is called on the executor after task execution and stored together with the used parameters in a log file; default: not set

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 *nameOfModuleType* and *substitutionGroup* set to *abstractTask*. Example 21 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 21: Assign a name to the module

```
1  <!-- make task definition available via substitution group -
->
2  <x:element name="nameOfModuleTask" type="nameOfModuleType"
substitutionGroup="abstractTask" />
3
4  <!-- definition of final task -->
5  <x:complexType name="nameOfModuleTaskType">
6    <x:complexContent>
7      <x:extension base="nameOfModuleTaskOverrideType">
8        <x:all>
9          <x:element name="parameter"
type="nameOfModuleTaskParameterType" minOccurs="1" maxOccurs="1"
/>
10         <x:element name="return"
type="nameOfModuleTaskReturnType" minOccurs="0" maxOccurs="0" />
11         <x:group ref="defaultTaskElements" />
12       </x:all>
13     </x:extension>
14   </x:complexContent>
15 </x:complexType>
```

5.5 Putting it all together

Example 22 shows the definition of the complete module.

Example 22: 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">
6          <x:all>
7              <x:element name="parameter1"
type="paramAbsolutePath" minOccurs="1" maxOccurs="1" />
8              <x:element name="parameter2"
type="paramString" minOccurs="0" maxOccurs="unbounded" />
9              <x:element name="flag1" type="paramBoolean"
minOccurs="0" maxOccurs="1" />
10             </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"
type="x:string" />
19                 </x:all>
20             </x:extension>
21         </x:complexContent>
22     </x:complexType>
23
24     <!-- set command and other settings -->
25     <x:complexType name="nameOfModuleTaskOverrideType">
26         <x:complexContent>
27             <x:restriction base="baseAttributeTaskType">
28                 <x:attribute name="binName"
type="x:string" fixed="nameOfModule.sh" />
29             </x:restriction>
30         </x:complexContent>
31     </x:complexType>
32
33     <!-- make task definition available via substitution
group -->
34     <x:element name="nameOfModuleTask"
type="nameOfModuleTaskType" substitutionGroup="abstractTask" />
35
36     <!-- definition of final task -->
37     <x:complexType name="nameOfModuleTaskType">
```

```

38         <x:complexContent>
39             <x:extension
base="nameOfModuleTaskOverrideType">
40                 <x:all>
41                     <x:element name="parameter"
type="nameOfModuleTaskParameterType" minOccurs="1" maxOccurs="1"
/>
42                     <x:element name="return"
type="nameOfModuleTaskReturnType" minOccurs="0" maxOccurs="0" />
43                     <x:group ref="defaultTaskElements"
/>
44                 </x:all>
45             </x:extension>
46         </x:complexContent>
47     </x:complexType>
48
49 </x:schema>

```

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 23 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 23: Rename of parameters

```

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="featureCountsTaskParameterType">
6          <x:all>
7              <!-- attributes common to all versions -->
8              ...

```

```

9
10         <!-- attributes that differ between versions
-->
11         <x:element name="minOverlap"
type="paramInteger" minOccurs="0" maxOccurs="1" maxVersion="1" />
12         <x:element name="minReadOverlap"
type="paramInteger" minOccurs="0" maxOccurs="1" minVersion="2" />
13         ...
14     </x:all>
15 </x:complexType>
16 ...
17 </x:schema>

```

Example 24 shows how a module script can be made version dependent using bash functions that are delivered with Watchdog. First, the bash variable `${MODULE_VERSION_PARAMETER_NAME}` is set to the complete name of the parameter that is used to pass the module version (e.g. `--moduleVersion`) (3). After sourcing of `includeBasics.sh` the module version is automatically stored in the `${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 24: Version dependent bash script

```

1  #!/bin/bash
2  SCRIPT_FOLDER=$( cd "$( dirname "${BASH_SOURCE[0]}" )" &&
pwd )
3  MODULE_VERSION_PARAMETER_NAME="--moduleVersion"
4  source $SCRIPT_FOLDER/../../core_lib/includeBasics.sh $@
5  ...
6
7  # define parameters
8  # params used in any version of the module
9  DEFINE_string 'annotation' '' 'feature annotation in GTF or
SAF format' 'a'
10 DEFINE_string 'input' '' 'index bam file which should be
used for counting' 'i'
11 DEFINE_string 'output' '' 'path to output file' 'o'
12 ...
13
14 # params only available in module version 1
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'
17 # params only available in module version 2
18 elif [ ${MODULE_VERSION} -eq 2 ]; then
19     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     ...
21     fi
22     DEFINE_integer 'moduleVersion' '1' '[optional] version of
the module that should be used' ''
23     DEFINE_boolean 'debug' 'false' '[optional] prints out debug
messages.' 'T'
24     ...

```

5.7 Requirements to support package manager wrappers

Currently, only the Conda package manager is supported as execution wrapper by the `<conda>` XML plugin. A module that should support the `<conda>` XML plugin must contain a [YAML file](#) defining the Conda environment.

Example 25: Conda environment file format

```

1     channels:
2         - bioconda
3         - conda-forge
4     dependencies:
5         - coreutils=8.31
6         - grep=2.14
7         - samtools=1.10
8         - sed=4.7

```

Example 25 shows the Conda environment file for the *indexBam* module.

The script *helper_scripts/formatCondaYaml.py* can be used to sort channels and dependencies alphabetically. This is important as only one Conda environment per file hash will be initialized and hence could reduce space usage if many modules depend on the same requirements.

5.8 Documentation of modules

Modules can be documented using an XML format that is defined by an XSD schema. Such an XML module documentation file consists of the main sections `<info>`, `<parameter>` and `<return>`. The first section is mandatory while the other two are optional (e.g. for modules that do not require any parameter or do not return variables).

Example 26: XML module documentation format

```

1     <?xml version="1.0" encoding="UTF-8"?>
2     <documentation xmlns:xsi="http://www.w3.org/2001/XMLSchema-
instance" xsi:noNamespaceSchemaLocation="documentation.xsd">

```

```

3      <!-- mandatory fields: author, category, updated,
description -->
4      <info>
5          <!-- forename lastname -->
6          <author>Michael Kluge</author>
7          <!-- day the module was updated the last time -->
8          <updated>2019-03-13</updated>
9          <category>Sequencing</category>
10         <description maxVersion="1" minVersion="1">creates an
index for a BAM file using samtools index</description>
11         <!-- ##### optional ##### -->
12         <!-- website of the dependencies used in this module -->
13         <website>https://www.htslib.org/doc/samtools.html</website>
14         <!-- short description and PubMedID for the methods
section of a manuscript -->
15         <paperDescription>Samtools (%SOFTWARE_VERSION%) was used
to index the BAM files [Li H, Handsaker B, Wysoker A, Fennell T,
Ruan J, Homer N, Marth G, Abecasis G, Durbin R, and 1000 Genome
Project Data Processing Subgroup, The Sequence alignment/map
(SAM) format and SAMtools, Bioinformatics (2009) 25(16) 2078-9].
</paperDescription>
16         <PMID>19505943</PMID>
17         <!-- external dependencies required for that module -->
18         <dependencies maxVersion="1"
minVersion="1">samtools</dependencies>
19         <dependencies maxVersion="1" minVersion="1">GNU Core
Utilities</dependencies>
20     </info>
21     <!-- ##### optional ##### -->
22     <!-- github usernames of users who should be able to
commit changes to that module -->
23     <maintainer>
24         <username>klugem</username>
25     </maintainer>
26     <parameter>
27         <!-- mandatory fields per parameter: name, type,
description -->
28         <!-- optional fields per parameter: restrictions,
default, minOccurs, maxOccurs, minVersion, maxVersion -->
29         <param maxOccurs="1" minOccurs="1" name="bam" type="file
path" restrictions="absolute">
30             <description>path to the BAM file</description>
31         </param>
32         <param default="true" maxOccurs="1" minOccurs="0"
name="link" type="boolean">
33             <description>creates a link called NAME.bam.bai
because some tool expect the index under that name; use --nolink
to disable it</description>
34         </param>
35     </parameter>
36     <return>

```

```

37      <!-- mandatory fields per return variable: name, type,
description -->
38      <!-- optional fields per return variable: minVersion,
maxVersion -->
39      <var name="BAMFile" type="string">
40          <description>path to the BAM file for which the index
was created</description>
41      </var>
42  </return>
43 </documentation>

```

Example 26 shows the XML documentation file for the *indexBam* module. The tag **<paperDescription>** (15), which is a child of **<info>**, allows to define the description used during report generation (see [6.3](#)). This description can also contain references to parameters of the task (*%param_name%*) or the software version (*%SOFTWARE_VERSION%*).

An XML template for documenting a new module can be generated based on the XSD module file using the *docuTemplateExtractor.jar* (see [6.1](#)). Hence, only some information must be updated or added manually.

5.9 Other matters

Exit codes: The module developer must ensure that a command does only exit with exit status 0 if the command was executed successfully. File *core_lib/exitCodes.sh* 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 *[ERROR]*. The errors are only stored if standard out and error files are saved to disk using the **<streams>** 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 New features in Watchdog 2.0

In the following the new command-line tools (available in the *jars/* subfolder of the Watchdog installation directory) are described in more detail. All tools can be executed using *java -jar path/to/jar/name.jar -options*. The available parameter and flags can be listed using *java -jar path/to/jar/name.jar -help*.

Information on module versioning can be found in section [5.6](#). The new XML plugin for execution wrappers is described in [4.4](#) and requirements modules must fulfil to be supported by the Conda package manager in [5.7](#). The documentation of the graphical user interface for module creation (*moduleMaker.jar*) has its own [documentation](#).

6.1 Documentation template extractor

The *docuTemplateExtractor* command-line tool can be used to extract parameter and return value information from XSD module files. The program then creates an XML documentation template file for each module in the corresponding module folder. By default existing XML documentation files of modules are not overwritten. This can be disabled with the *-overwrite* flag. Using the *-authors*, *-maintainer* or *-categories* parameter, the same author, maintainer or categories can be included in all created template files.

Example call:

```
java -jar docuTemplateExtractor.jar -moduleFolder  
/path/to/watchdog/modules
```

Moreover, custom extractor plugins can be implemented to extract additional information like default parameters or descriptions. Currently, parameter extractors for the python *argparse* and the Bash *shflags* library are available. Additional custom extractors can be added by implementing the Java *Extractor* interface of the *de.lmu.ipi.bio.watchdog.docu.extractor* package. Afterwards a compiled class file must be added to *docuTemplateExtractor*, which can be edited with any ZIP editor. The tool will automatically detected all classes implementing the *Extractor* interface.

Information on the module XML documentation format itself can be found in section [5.8](#).

6.2 Module reference book generator

The module reference book can be created from the XML documentation files using the *refBookGenerator* command-line tool.

One ore more path to the parent folder(s) of modules that should be included in the module reference book must be provided using the *-moduleFolder* parameter. Moreover, a path to a folder, in which the module reference book should be stored, must be specified using the *-outputFolder* parameter.

Example call:

```
java -jar refBookGenerator.jar -moduleFolder  
/path/to/watchdog/modules -moduleFolder /tmp/customModules -  
outputFolder /tmp/refBook
```

6.3 Report generator

A report of the executed steps of a workflow can be automatically created using the *reportGenerator* command-line tool. In order to generate a report, these three parameters are required:

- -resume: path to watchdog status log file (alias resume file) from a previous Watchdog run
- -xml: path to the XML workflow file (required for loading the correct module folders)
- -outputFile: path to an output file in which the resulting report is stored as text

Example call:

```
java -jar reportGenerator.jar -xml /path/to/wf1.xml -resume  
/path/to/wf1_2019_11_07_11_48_26.watchdog.resume -outputFile  
/tmp/report.txt
```

Additional parameters exist to enable or suppress the output of some information or to modify the output format. The available parameters can be listed using the *-help* flag.

6.4 Module and workflow validator

The module (*moduleValidator*) and workflow (*workflowValidator*) validators can be used to verify the integrity of modules or workflows respectively.

Both tools require as input the name of a check to perform (parameter *-check*) and a folder to apply the check onto (parameter *-folder*). Please note that only one module or workflow can be located in the folder. Names of checks that can be performed can be listed using the *-list* flag.

Example call:

```
java -jar moduleValidator.jar -check XSD_VALIDATION -folder  
/path/to/watchdog/modules/sleep
```

Additional information on the function of the applied checks can be found online at [watchdog-wms-modules](#) and [watchdog-wms-workflows](#).

6.5 Module and workflow repositories

Watchdog 2.0 now provides two repositories on Github under the [watchdog-wms organization](#) that are dedicated for sharing [modules](#) and [workflows](#), respectively, by other users.

6.6 New execution modes

Two additional execution modes were implemented to provide more comfort and flexibility in workflow execution.

The resume mode allows restarting execution of a workflow by (re-)running only tasks that previously did not run (successfully) or were added or modified compared to the original execution. With Watchdog 2.0 each execution of a workflow creates a *.resume file that contains information on successfully finished tasks. With that file the *-resume* parameter of the Watchdog scheduler can be used to resume the execution of an aborted or modified workflow.

Example call:

```
./watchdog.sh -xml /path/to/wf1.xml -resume  
/path/to/wf1_2019_11_07_11_48_26.watchdog.resume
```

The second mode allows detaching the scheduler from workflow execution without aborting tasks running on a computer cluster and reattaching to execution at a later time and/or a different computer. A detach can be requested by pressing CTRL+C during workflow execution with the command-line version. The GUI provides a button to request a detach. A successful detach results in an *.attach file, which can be used to reattach to workflow execution with the new *-attachInfo* parameter of the Watchdog scheduler.

Example call:

```
./watchdog.sh -xml /path/to/wf1.xml -attachInfo  
/path/to/wf1_2019_11_07_11_48_26.watchdog.attach
```

6.7 Software version logging

Watchdog 2.0 now implements a general approach for reporting versions of third-party software used in a module in the log file. For this purpose, a new attribute (*versionQueryParameter*) in the module XSD file can be used to define the flag for version printing of third-party software (see [5.3](#)). During workflow execution, after a task or subtask has been completed successfully on a particular computer, the program call defined in the corresponding module is invoked with the version flag on the same computer to retrieve the installed third-party software version. This software version is then reported for the task/subtask in the log file and can also be used during report generation (see [5.8](#) and [6.3](#)).

7 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 [7.1](#))
- *XML Plugins* that add new `<?Executor>` and `<?ProcessBlock>` elements (see [7.2](#))

7.1 Virtual file systems for task actions

With the help of task actions, file system operations can be performed before and after tasks (see [4.9](#)). 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 added 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
- *getExtensions* - sets schemes that should be used for specific file extension

The class *SimpleVFSRegister* can be extended if an instance of the *FileProvider* class can be created without arguments. Then only the name of the *FileProvider* class and the URL schemes that should be used must be defined. Example 27 shows how the virtual FTP file system is integrated in Watchdog by using the *FtpsFileProvider* class of the Commons Virtual File System project.

Example 27: Simple implementation of the VFSRegister interface

```
1 package de.lmu.ifi.bio.watchdog.task.actions.vfs.impl;
2
3 public class FTPSVFSRegister extends SimpleVFSRegister {
4
5     private static final String CLASS_NAME =
"org.apache.commons.vfs2.provider.ftp.FtpsFileProvider";
6     private static final String[] SCHEME = new String[]
{"ftp"};
7
8     public FTPSVFSRegister() throws Exception {
```



```

9         super(CLASS_NAME, SCHEME);
10     }
11 }

```

7.2 XML Plugins

Watchdog provides a flexible plugin system that allows extending Watchdog by additional types of executors, process blocks, and execution wrappers 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 *XMLParserPlugin* abstract class are loaded dynamically during workflow execution. Currently, this is restricted to XML parsers for the generic type *ProcessBlock*, *ExecutorInfo*, and *ExecutionWrapper*. The XML parser for a new XML element provides the functionality to parse this element in a workflow (i.e. a new executor, process block type, or execution wrapper) and to create a new object representing the corresponding element type. Here, the four most important functions of the *XMLParserPlugin* 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 *XMLDataStore* and *XMLPlugin*, for instance by extending one of the abstract classes *ProcessBlock*, *ExecutorInfo*, *ExecutionWrapper*, 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 *PluginView* and *PluginViewController* have to be implemented for testing whether the input is valid and for loading and saving data to and from XML.

All executors, process blocks, and execution wrapper 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](#).

8 Docker

In order to run a Docker image, Docker must be installed and configured correctly as described [here](#).

8.1 Install the Watchdog Docker image

A Watchdog image for Docker can be obtained from hub.docker.com. The image is rebuilt automatically by the Bioconda project once a new version is released on [Bioconda](#).

You can download the latest version 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.

8.2 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.

```
docker run -v source_folder_or_file_on_host:destination_folder_or_file[:ro] image command
```

More information can be found in the [documentation](#) of Docker.

8.3 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 [documentation](#) of Docker.

8.4 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 [3.2](#) 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 [8.2](#). Ensure that all files used in the workflow are made accessible within the Docker image.

To start the workflow designer GUI, run docker in interactive mode and allow it to connect to the local Xserver:

```
docker run -e DISPLAY=$DISPLAY -v /tmp/.X11-unix:/tmp/.X11-unix -it klugem/watchdog-wms /bin/bash
```

Then you can use *watchdog-gui* to start the workflow designer.

8.5 Use Docker in modules

A Docker image can also be used in a module. The module *bowtie2Docker* implements an example module that uses the Docker image of [Bowtie 2](#) that is provided by [Bioconda](#) and hosted on [quay.io](#). 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 28: Example usage of the Bowtie 2 Docker module

```
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      <settings>
5          <constants>
6              <const name="BASE">
{%INSTALL%}/modules/bowtie2Docker/example_data</const>
7              </constants>
8          </settings>
9
10         <tasks mail="{%MAIL%}">
11             <bowtie2DockerTask id="1"
name="bowtie2_in_docker">
12                 <streams>
13
14 <stdout>/tmp/bowtie2.docker.test.out</stdout>
15 <stderr>/tmp/bowtie2.docker.test.err</stderr>
16                 </streams>
17             </parameter>
```

```

17 <genome>${BASE}/index/lambda_virus</genome>
18         <reads>${BASE}/reads/reads_1.fq</reads>
19         <reads>${BASE}/reads/reads_1.fq</reads>
20 <outfile>/tmp/bowtie2.docker.test.sam</outfile>
21         </parameter>
22     </bowtie2DockerTask>
23 </tasks>
24 </watchdog>

```

Example 28 shows how the *bowtie2Docker* module can be used with the provided example data. The test data that is shipped with Bowtie 2 is stored in the folder *example_data* of the module (6). Log files are written to */tmp/bowtie2.docker.test.[out|err]* (13, 14) while the mapped reads are stored in SAM format in */tmp/bowtie2.docker.test.sam* (20).