

JUBE Documentation

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CHAPTER

ONE

INTRODUCTION

Automating benchmarks is important for reproducibility and hence comparability which is the major intent when performing benchmarks. Furthermore managing different combinations of parameters is error-prone and often results in significant amounts of work especially if the parameter space gets large.

In order to alleviate these problems *JUBE* helps performing and analyzing benchmarks in a systematic way. It allows custom work flows to be able to adapt to new architectures.

For each benchmark application the benchmark data is written out in a certain format that enables *JUBE* to deduct the desired information. This data can be parsed by automatic pre- and post-processing scripts that draw information, and store it more densely for manual interpretation.

The *JUBE* benchmarking environment provides a script based framework to easily create benchmark sets, run those sets on different computer systems and evaluate the results. It is actively developed by the Jülich Supercomputing Centre of Forschungszentrum Jülich, Germany.

JUBE TUTORIAL

This tutorial is meant to give you an overview about the basic usage of JUBE.

2.1 Installation

Requirements: JUBE needs Python 3.2 (or any higher version)

If you plan to use YAML based JUBE input files, you have to add the pyyaml-module to your Python module library.

To use the *JUBE* command line tool, the PYTHONPATH must contain the position of the *JUBE* package. This can be achieved in different ways:

• You can use the **installation script** to copy all files to the right position (preferred):

```
>>> python setup.py install --user
```

This will install the *JUBE* package files and executables to your \$HOME/.local directory. Instead of —user also a user specific —prefix option is available. Here you might have to set the PYTHONPATH environment variable first (this will be mentioned during the install process).

• You can utilize pip[3] to take care of the installation process (including the download)

```
>>> pip3 install http://apps.fz-juelich.de/jsc/jube/jube2/download.php?

version=latest --user

or
>>> pip3 install http://apps.fz-juelich.de/jsc/jube/jube2/download.php?

version=latest --prefix=...
```

You might have to adjust your PYTHONPATH.

• You can add the **parent folder path** of the *JUBE* package-folder (jube2 directory) to the PYTHONPATH environment variable:

```
>>> export PYTHONPATH=<parent folder path>: $PYTHONPATH
```

• You can move the JUBE package by hand to an existing Python package folder like site-packages

To use the *JUBE* command line tool like a normal command line command you can add it to the PATH environment variable:

```
>>> export PATH=$HOME/.local/bin:$PATH
```

To check your final installation, you can use

```
>>> jube --version
```

which should highlight the current version number.

2.2 Configuration

The main *JUBE* configuration bases on the given input configuration file. But in addition, some shell environment variables are available which can be used to set system specific options:

- JUBE_INCLUDE_PATH: Can contain a list of paths (seperated by :) pointing to directories, which contain system relevant include configuration files. This technique can be used to store platform specific parameter in a platform specific directory.
- JUBE_EXEC_SHELL: *JUBE* normally uses /bin/sh to execute the given shell commands. This default shell can be changed by using this environment variable.
- JUBE_GROUP_NAME: JUBE will use the given UNIX groupname to share benchmarks between different users. The group must exist and the JUBE user must be part of this group. The given group will be the owner of new benchmark runs. By default (without setting the environment variable) all file and directory permissions are defined by the normal UNIX rules.

BASH autocompletion can be enabled by using the eval "\$(jube complete)" command. You can store the command in your bash profile settings if needed.

2.3 Input format

JUBE supports two different types of input formats: XML based files and YAML based files. Both formats support the same amount of JUBE features and you can select your more preffered input format.

The following sections will always show all examples using both formats. However the explanations will mostly stick to the *XML* format but can be easily transferred to the *YAML* solution.

Both formats depends on a specifc special scharacter handling. More details can be found in the following FAQ sections:

- XML character handling
- YAML character handling

Internally *JUBE* always uses the *XML* based format, by converting *YAML* based configuration files into *XML* if necessary. This is why parsing error messages might point to *XML* errors even if the *YAML* format was used.

2.4 Hello World

In this example we will show you the basic structure of a JUBE input file and the basic command line options.

The files used for this example can be found inside examples/hello_world.

The input file hello world.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="hello_world" outpath="bench_run">
       <comment>A simple hello world
4
5
       <!-- Configuration -->
6
       <parameterset name="hello_parameter">
         <parameter name="hello_str">Hello World</parameter>
       </parameterset>
10
       <!-- Operation -->
11
       <step name="say_hello">
12
         <use>hello_parameter</use> <!-- use existing parameterset -->
13
         <do>echo $hello_str</do> <!-- shell command -->
```

The input file hello_world.yaml:

```
name: hello_world
   outpath: bench_run
   comment: A simple hello world
   #Configuration
   parameterset:
6
     name: hello_parameter
     parameter: {name: hello_str, _: Hello World}
8
   #Operation
10
11
   step:
12
     name: say_hello
13
     use: hello_parameter #use existing parameter
     do: echo $hello_str #shell command
```

Every *JUBE XML* based input file starts (after the general *XML* header line) with the root tag < jube>. This root tag must be unique. *XML* does not allow multiple root tags.

The first tag which contains benchmark specific information is <benchmark>. hello_world is the benchmarkname which can be used to identify the benchmark (e.g. when there are multiple benchmarks inside a single input file, or when different benchmarks use the same run directory).

The outpath describes the benchmark run directory (relative to the position of the input file). This directory will be managed by *JUBE* and will be automatically created if it does not exist. The directory name and position are very important, because they are the main interface to communicate with your benchmark, after it was submitted.

Using the <comment> you can store some benchmark related comments inside the benchmark directory. You can also use normal *XML*-comments to structure your input-file:

```
<!-- your comment -->
```

In this benchmark a <parameterset> is used to store the single <parameter name="hello_str">.
The name of the parameter should contain only letters, numbers (should not be the first character) or the _ (like a normal *Python* identifier). The name of the parameterset must be unique (relative to the current benchmark). In further examples we will see that there are more types of sets, which can be distinguished by their names. Also the name of the parameter must be unique (relative to the parameterset).

The <step> contains the operation tasks. The name must be unique. It can use different types of existing sets. All used sets must be given by name using the <use>. There can be multiple <use> inside the same <step> and also multiple names within the same <use> are allowed (separated by ,). Only sets, which are explicitly used, are available inside the step! The <do> contains a single **shell command**. This command will run inside of a sandbox directory environment (inside the outpath directory tree). The step and its corresponding *parameter space* is named *workpackage*.

Available parameters can be used inside the shell commands. To use a parameter you have to write

```
$parametername
```

or

```
${parametername}
```

The brackets must be used if you want variable concatenation. \$hello_strtest will not be replaced, \${hello_str}test will be replaced. If a parameter does not exist or isn't available the variable will not be replaced! If you want to use \$ inside your command, you have to write \$\$ to mask the symbol. Parameter substitution will be done before the normal shell substitution!

2.4. Hello World 5

To run the benchmark just type:

```
>>> jube run hello_world.xml
```

This benchmark will produce the follwing output:

```
# benchmark: hello_world
  # id: 0
  # A simple hello world
5
  Running workpackages (#=done, 0=wait, E=error):
  10
11
   | stepname | all | open | wait | error | done |
   |----|---|----|
12
   | say_hello | 1 | 0 | 0 | 0 |
13
14
  >>>> Benchmark information and further useful commands:
15
     id: 0
16
  >>>>
      handle: bench_run
17
  >>>>
      dir: bench_run/000000
18
  >>>> analyse: jube analyse bench_run --id 0
19
     result: jube result bench_run --id 0
20
 >>>>
      info: jube info bench_run --id 0
 >>>>
21
       log: jube log bench_run --id 0
 >>>>
22
```

As you can see, there was a single step say_hello, which runs one shell command echo \$hello_str that will be expanded to echo Hello World.

The **id** is (in addition to the benchmark directory handle) an important number. Every benchmark run will get a new unique **id** inside the benchmark directory.

Inside the benchmark directory you will see the follwing structure:

```
# the given outpath
   bench_run
2
   +- 000000
                           # the benchmark id
3
4
      +- configuration.xml # the stored benchmark configuration
5
      +- workpackages.xml # workpackage information
6
      +- run.log
                            # log information
7
      +- 000000_say_hello # the workpackage
8
         +- done
                           # workpackage finished marker
10
         +- work
                           # user sandbox folder
11
12
            +- stderr
                          # standard error messages of used shell commands
13
            +- stdout
                           # standard output of used shell commands
14
```

stdout will contain Hello World in this example case.

2.5 Help

JUBE contains a command line based help functionality:

```
>>> jube help <keyword>
```

By using this command you will have direct access to all keywords inside the *glossary*.

Another useful command is the info command. It will show you information concerning your existing benchmarks:

```
# display a list of existing benchmarks

>>> jube info <benchmark-directory>
# display information about given benchmark

>>> jube info <benchmark-directory> -- id <id>
# display information about a step inside the given benchmark

>>> jube info <benchmark-directory> -- id <id> --step <stepname>
```

The third, also very important, functionality is the **logger**. Every run, continue, analyse and result execution will produce log information inside your benchmark directory. This file contains much useful debugging output.

You can easily access these log files by using the JUBE log viewer command:

```
>>> jube log [benchmark-directory] [--id id] [--command cmd]
```

e.g.:

```
>>> jube log bench_runs --command run
```

will display the run.log of the last benchmark found inside of bench_runs.

Log output can also be displayed during runtime by using the verbose output:

```
>>> jube -v run <input-file>
```

-vv can be used to display stdout output during runtime and -vvv will display the stdout output as well as the log output at the same time.

Since the parsing step is done before creating the benchmark directory, there will be a jube-parse.log inside your current working directory, which contains the parser log information.

Errors within a <do> command will create a log entry and stop further execution of the corresponding parameter combination. Other parameter combinations will still be executed by default. *JUBE* can also stop automatically any further execution by using the -e option:

```
>>> jube run -e <input-file>
```

There is also a debugging mode integrated in *JUBE*:

```
>>> jube --debug <command> [other-args]
```

This mode avoids any *shell* execution but will generate a single log file (jube-debug.log) in your current working directory.

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2.6 Parameter space creation

In this example we will show you an important feature of JUBE: The automatic parameter space generation.

The files used for this example can be found inside examples/parameterspace.

The input file parameterspace.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
     <benchmark name="parameterspace" outpath="bench_run">
       <comment>A parameterspace example
       <!-- Configuration -->
       <parameterset name="param_set">
         <!-- Create a parameterspace out of two template parameter -->
         <parameter name="number" type="int">1,2,4</parameter>
         <parameter name="text" separator=";">Hello;World</parameter>
10
11
       </parameterset>
12
13
       <!-- Operation -->
       <step name="say_hello">
14
         <use>param_set</use> <!-- use existing parameterset -->
15
         <do>echo "$text $number"</do> <!-- shell command -->
16
17
       </step>
18
     </benchmark>
   </jube>
```

The input file parameterspace.yaml:

```
name: parameterspace
   outpath: bench_run
   comment: A parameterspace example
   #Configuration
   parameterset:
     name: param set
     #Create a parameterspace out of two template parameter
       - {name: number, type: int, _: "1,2,4"} #comma separated integer must be quoted
       - {name: text, separator: ;, _: Hello; World}
11
12
13
   #Operation
14
   step:
     name: say_hello
15
     use: param_set #use existing parameterset
16
     do: echo "$text $number" #shell command
17
```

Whenever a parameter contains a , (this can be changed using the separator attribute) this parameter becomes a **template**. A step which **uses the parameterset** containing this parameter will run multiple times to iterate over all possible parameter combinations. In this example the step say_hello will run 6 times:

Every parameter combination will run in its own sandbox directory.

Another new keyword is the type attribute. The parameter type is not used inside the substitution process, but for sorting operations inside the result creation. The default type is string. Possible basic types are string, int and float.

2.7 Step dependencies

If you start writing a complex benchmark structure, you might want to have dependencies between different *steps*, for example between a compile and the execution step. *JUBE* can handle these dependencies and will also preserve the given *parameter space*.

The files used for this example can be found inside examples/dependencies.

The input file dependencies.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
2
     <benchmark name="dependencies" outpath="bench_run">
       <comment>A Dependency example
       <!-- Configuration -->
       <parameterset name="param_set">
         <parameter name="number" type="int">1,2,4</parameter>
       </parameterset>
10
       <!-- Operations -->
11
       <step name="first_step">
12
         <use>param_set</use> <!-- use existing parameterset -->
13
         <do>echo $number</do> <!-- shell command -->
       </step>
15
16
17
       <!-- Create a dependency between both steps -->
       <step name="second_step" depend="first_step">
18
         <do>cat first_step/stdout</do> <!-- shell command -->
19
       </step>
20
     </benchmark>
21
   </jube>
```

The input file dependencies.yaml:

```
name: dependencies
   outpath: bench_run
   comment: A Dependency example
   #Configuration
   parameterset:
     name: param_set
     parameter: {name: number, type: int, _: "1,2,4" } #comma separated integers_
   →must be quoted
   #Operation
10
11
   step:
     - name: first_step
12
       use: param_set #use existing parameterset
13
       do: echo $number #shell command
14
15
     - name: second_step
       depend: first_step #Create a dependency between both steps
16
       do: cat first_step/stdout #shell command
17
```

In this example we create a dependency between first_step and second_step. After first_step is finished, the corresponding second_step will start. Steps can also have multiple dependencies (separated by , in the definition), but circular definitions will not be resolved. A dependency is a unidirectional link!

To communicate between a step and its dependency there is a link inside the work directory pointing to the corresponding dependency step work directory. In this example we use

```
cat first_step/stdout
```

to write the stdout-file content of the dependency step into the stdout-file of the current step.

Because the first_step uses a template parameter which creates three execution runs, there will also be three second_step runs each pointing to different first_step-directories:

2.8 Loading files and substitution

Every step runs inside a unique sandbox directory. Usually, you will need to have external files inside this directory (e.g. the source files) and in some cases you want to change a parameter inside the file based on your current *parameter space*. There are two additional set-types which handle this behaviour inside of *JUBE*.

The files used for this example can be found inside examples/files_and_sub.

The input file files_and_sub.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="files_and_sub" outpath="bench_run">
3
       <comment>A file copy and substitution example
4
5
6
       <!-- Configuration -->
       <parameterset name="param_set">
         <parameter name="number" type="int">1,2,4</parameter>
       </parameterset>
10
       <!-- Files -->
11
       <fileset name="files">
12
         <copy>file.in</copy>
13
       </fileset>
14
15
       <!-- Substitute -->
16
       <substituteset name="substitute">
17
         <!-- Substitute files -->
18
         <iofile in="file.in" out="file.out" />
19
20
         <!-- Substitute commands -->
         <sub source="#NUMBER#" dest="$number" />
21
       </substituteset>
22
23
       <!-- Operation -->
24
       <step name="sub_step">
25
         <use>param_set</use> <!-- use existing parameterset -->
26
         <use>files</use>
                                <!-- use existing fileset -->
27
         <use>substitute</use> <!-- use existing substituteset -->
28
         <do>cat file.out</do> <!-- shell command -->
29
       </step>
30
     </benchmark>
31
   </jube>
32
```

The input file files_and_sub.yaml:

```
name: files_and_sub
outpath: bench_run
comment: A file copy and substitution example

#Configuration
parameterset:
```

```
name: param_set
     parameter: {name: number, type: int, _: "1,2,4"} #comma separated integers must_
8
    →be quoted
   #Files
10
   fileset:
11
     name: files
12
     copy: file.in
13
14
   #Substitute
15
   substituteset:
16
     name: substitute
17
     iofile: {in: file.in, out: file.out}
18
     sub: {source: "#NUMBER#", dest: $number} #"#" must be quoted
19
20
21
   #Operation
22
   step:
     name: sub_step
23
     use:
24
        - param_set #use existing parameterset
25
        - files #use existing fileset
26
        - substitute #use existing substituteset
27
     do: cat file.out #shell command
```

The content of file file.in:

```
Number: #NUMBER#
```

Inside the <fileset> the current location (relative to the current input file; also absolute paths are allowed) of files is defined. <copy> specifies that the file should be copied to the sandbox directory when the fileset is used. Also a a vailable to create a symbolic link to the given file inside the sandbox directory.

If there are additional operations needed to *prepare* your files (e.g. expand a tar-file). You can use the <p

The <substituteset> describes the substitution process. The <iofile> contains the input and output filename. The path is relative to the sandbox directory. Because we do/should not know that location we use the fileset to copy file.in to this directory.

The <sub> specifies the substitution. All occurrences of source will be substituted by dest. As you can see, you can use parameters inside the substitution.

There is no <use> inside any set. The combination of all sets will be done inside the <step>. So if you use a parameter inside a <sub> you must also add the corresponding <parameterset> inside the <step> where you use the <substituteset>!

In the sub_step we use all available sets. The use order is not relevant. The normal execution process will be:

- 1. Parameter space expansion
- 2. Copy/link files
- 3. Prepare operations
- 4. File substitution
- 5. Run shell operations

The resulting directory-tree will be:

```
+- configuration.xml # the stored benchmark configuration
      +- workpackages.xml # workpackage information
6
      +- 000000_sub_step \# the workpackage ($number = 1)
         +- done
                            # workpackage finished marker
                            # user sandbox folder
10
         +- work
11
                           # standard error messages of used shell commands
            +- stderr
12
                            # standard output of used shell commands (Number: 1)
            +- stdout
13
            +- file.in
                           # the file copy
14
            +- file.out
                            # the substituted file
15
      +- 000001_sub_step
                          # the workpackage ($number = 2)
16
17
18
         +- ...
```

2.9 Creating a result table

Finally, after running the benchmark, you will get several directories. *JUBE* allows you to parse your result files distributed over these directories to extract relevant data (e.g. walltime information) and create a result table.

The files used for this example can be found inside examples/result_creation.

The input file result_creation.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="result_creation" outpath="bench_run">
3
       <comment>A result creation example
4
5
       <!-- Configuration -->
6
       <parameterset name="param_set">
         <!-- Create a parameterspace with one template parameter -->
         <parameter name="number" type="int">1,2,4</parameter>
10
       </parameterset>
11
       <!-- Regex pattern -->
12
       <patternset name="pattern">
13
         <pattern name="number_pat" type="int">Number: $jube_pat_int</pattern>
14
       </patternset>
15
16
       <!-- Operation -->
17
       <step name="write_number">
18
         <use>param_set</use> <!-- use existing parameterset -->
19
         <do>echo "Number: $number"</do> <!-- shell command -->
20
       </step>
21
22
       <!-- Analyse -->
23
       <analyser name="analyse">
24
         <use>pattern</use> <!-- use existing patternset -->
25
         <analyse step="write_number">
26
           <file>stdout</file> <!-- file which should be scanned -->
27
28
         </analyse>
       </analyser>
29
30
       <!-- Create result table -->
31
       <result>
32
         <use>analyse <!-- use existing analyser -->
33
         34
```

The input file result_creation.yaml:

```
name: result_creation
   outpath: bench_run
2
   comment: A result creation example
3
4
   #Configuration
5
   parameterset:
6
     name: param_set
      #Create a parameterspace with one template parameter
     parameter: {name: number, type: int, _: "1,2,4"} #comma separated integer must_
    →be quoted
10
   #Regex pattern
11
   patternset:
12
     name: pattern
13
     pattern: {name: number_pat, type: int, _: "Number: $jube_pat_int"} # ":" must be_
14
    \hookrightarrowquoted
15
   #Operation
16
   step:
17
     name: write_number
18
19
     use: param_set #use existing parameterset
     do: 'echo "Number: $number"' #shell command
20
21
   #Analvse
22
   analyser:
23
     name: analyse
24
25
     use: pattern #use existing patternset
     analyse:
26
        step: write_number
27
        file: stdout #file which should be scanned
28
29
   #Create result table
30
   result:
31
     use: analyse #use existing analyser
32
     table:
33
       name: result
34
       style: pretty
35
        sort: number
36
        column: [number, number_pat]
```

Now we want to parse these stdout files to extract information (in this example case the written number). First of all we have to declare a <patternset>. Here we can describe a set of <pattern>. A <pattern> is a regular expression which will be used to parse your result files and search for a given string. In this example we only have the <pattern> number_pat. The name of the pattern must be unique (based on the usage of the <patternset>). The type is optional. It is used when the extracted data will be sorted. The regular expression can contain other patterns or parameters. The example uses \$jube_pat_int which is a JUBE default pattern matching integer values. The pattern can contain a group, given by brackets (...), to declare the extraction part (\$jube_pat_int already contains these brackets).

E.g. \$jube_pat_int and \$jube_pat_fp are defined in the following way:

```
<pattern name="jube_pat_int" type="int">([+-]?\d+)</pattern>
<pattern name="jube_pat_fp" type="float">([+-]?\d*\.?\d+(?:[eE][-+]?\d+)?)</pattern>
```

If there are multiple matches inside a single file you can add a *reduce option*. By default, only the first match will be extracted.

To use your <patternset> you have to specify the files which should be parsed. This can be done using the <analyse>. It uses relevant patternsets. Inside the <analyse> a step-name and a file inside this step is given. Every workpackage file combination will create its own result entry.

The analyser automatically knows all parameters which were used in the given step and in depending steps. There is no <use> option to include additional <parameterset> that have not been already used within the analysed <step>.

To run the anlayse you have to write:

```
>>> jube analyse bench_run
```

The analyse data will be stored inside the benchmark directory.

The last part is the result table creation. Here you have to use an existing analyser. The <column> contains a pattern or a parameter name. sort is the optional sorting order (separated by ,). The style attribute can be csv, pretty or aligned to get different ASCII representations.

To create the result table you have to write:

```
>>> jube result bench_run -i last
```

If you run the result command for the first time, the analyse step will be executed automatically, if it wasn't executed before. So it is not necessary to run the separate analyse step all the time. However you need the separate analyse if you want to force a re-run of the analyse step, otherwise only the stored values of the first analyse will be used in the result step.

The result table will be written to STDOUT and into a result.dat file inside bench_run/<id>/result. The last is the default option and can also be replaced by a specific benchmark id. If the id selection is missing a combined result table of all available benchmark runs from the bench_run directory will be created.

Output of the given example:

The analyse and result instructions can be combined within one single command:

```
>>> jube result bench_run -a
```

This was the last example of the basic *JUBE* tutorial. Next you can start the *advanced tutorial* to get more information about including external sets, jobsystem representation and scripting parameter.

ADVANCED TUTORIAL

This tutorial demonstrates more detailed functions and tools of *JUBE*. If you want a basic overview you should read the general *JUBE tutorial* first.

3.1 Schema validation

To validate your XML based input files you can use DTD or schema validation. You will find jube.dtd, jube. xsd and jube.rnc inside the schema folder. You have to add these schema information to your input files which you want to validate.

DTD usage:

Schema usage:

RELAX NG Compact Syntax (RNC for emacs nxml-mode) usage:

In order to use the provided rnc schema file schema/jube.rnc in emacs open an xml file and use C-c C-s C-f or M-x rng-set-schema-file-and-validate to choose the rnc file. You can also use M-x customize-variable rng-schema-locating-files after you loaded nxml-mode to customize the default search paths to include jube.rnc. After successful parsing emacs offers to automatically create a schema.xml file which looks like

The next time you open the same xml file emacs will find the correct rnc for the validation based on schema.xml.

Example validation tools:

- eclipse (using DTD or schema)
- emacs (using RELAX NG)
- xmllint:
 - For validation (using the DTD):

```
>>> xmllint --noout --valid <xml input file>
```

- For validation (using the DTD and Schema):

```
>>> xmllint --noout --valid --schema <schema file> <xml input file>
```

3.2 Scripting parameter

In some cases it is needed to create a parameter which is based on the value of another parameter. In this case you can use a scripting parameter.

The files used for this example can be found inside examples/scripting_parameter.

The input file scripting_parameter.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
     <benchmark name="scripting_parameter" outpath="bench_run">
       <comment>A scripting parameter example</comment>
       <!-- Configuration -->
       <parameterset name="param_set">
          <!-- Normal template -->
         <parameter name="number" type="int">1,2,4</parameter>
          <!-- A template created by a scripting parameter-->
10
         <parameter name="additional_number" mode="python" type="int">
11
            ",".join(str(a*${number}) for a in [1,2])
12
13
         </parameter>
          <!-- A scripting parameter -->
14
         <parameter name="number_mult" mode="python" type="float">
15
            ${number}*${additional_number}
16
17
          </parameter>
          <!-- Reuse another parameter -->
18
          <parameter name="text">Number: $number</parameter>
19
       </parameterset>
20
21
       <!-- Operation -->
22
       <step name="operation">
23
          <use>param_set</use> <!-- use existing parameterset -->
24
          <!-- shell commands -->
25
         <do>echo "number: $number, additional_number: $additional_number"</do>
26
         <do>echo "number_mult: $number_mult, text: $text"</do>
27
       </step>
28
     </benchmark>
29
   </jube>
30
```

The input file scripting_parameter.yaml:

```
name: scripting_parameter

outpath: bench_run

comment: A scripting parameter example

#Configuration

parameterset:

name: param_set

parameter:

#Normal template

- {name: number, type: int, _: "1,2,4"}

#A template created by a scripting parameter

- {name: additional_number, mode: python, type: int, _: '",".join(str(a*$

→{number}) for a in [1,2])'}

(continues on next page)
```

```
#A scripting parameter
13
       - {name: number_mult, mode: python, type: float, _: "${number}*${additional_
14
    →number}"}
       #Reuse another parameter
15
       - {name: text, _: "Number: $number"}
17
18
   #Operation
19
   step:
     name: operation
20
     use: param_set #use existing parameterset
21
22
       - 'echo "number: $number, additional_number: $additional_number"'
23
       - 'echo "number_mult: $number_mult, text: $text"'
24
```

In this example we see four different parameters.

- number is a normal template which will be expanded to three different workpackages.
- additional_number is a scripting parameter which creates a new template and bases on number. The mode is set to the scripting language (python, perl and shell are allowed). The additional type is optional and declares the result type after evaluating the expression. The type is only used by the sort algorithm in the result step. It is not possible to create a template of different scripting parameters. Because of this second template we will get six different workpackages.
- number_mult is a small calculation. You can use any other existing parameters (which are used inside the same step).
- text is a normal parameter which uses the content of another parameter. For a simple concatenation parameter you do not need a scripting parameter.

For this example we will find the following output inside the run.log-file:

```
===== operation =====
   >>> echo "number: 1, additional_number: 1"
2
   >>> echo "number_mult: 1, text: Number: 1"
   ===== operation =====
  >>> echo "number: 1, additional_number: 2"
  >>> echo "number_mult: 2, text: Number: 1"
   ===== operation =====
   >>> echo "number: 2, additional_number: 2"
   >>> echo "number_mult: 4, text: Number: 2"
   ===== operation =====
10
   >>> echo "number: 2, additional_number: 4"
11
   >>> echo "number_mult: 8, text: Number: 2"
12
   ===== operation =====
13
   >>> echo "number: 4, additional_number: 4"
14
   >>> echo "number_mult: 16, text: Number: 4"
15
    ===== operation =====
16
   >>> echo "number: 4, additional_number: 8"
   >>> echo "number_mult: 32, text: Number: 4"
```

Implicit Perl or Python scripting inside the <do> or any other position is not possible. If you want to use some scripting expressions you have to create a new parameter.

3.3 Scripting pattern

Similar to the *Scripting parameter*, also different patterns, or patterns and parameters can be combined. For this a scripting pattern can be created by using the mode= attribute in the same way as it is used for the *Scripting parameter*.

All scripting patterns are evaluated at the end of the analyse part. Each scripting pattern is evaluated once. If there are multiple matches as described in the *Statistic pattern values* section, only the resulting statistical pattern is available (not each individual value). Scripting pattern do not create statistic values by themselves.

In addition the default = attribute can be used to set a default pattern value, if the value can't be found during the analysis.

The files used for this example can be found inside examples/scripting_pattern.

The input file scripting_pattern.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="scripting_pattern" outpath="bench_run">
       <comment>A scripting_pattern example</comment>
        <!-- Configuration -->
       <parameterset name="param_set">
          <parameter name="value" type="int">0,1,2</parameter>
        </parameterset>
10
        <!-- Operation -->
11
        <step name="operation">
12
          <use>param_set</use>
13
          <do>echo "$value"</do>
14
        </step>
15
16
17
        <!-- Pattern to extract -->
        <patternset name="pattern_set">
18
          <!-- A normal pattern -->
19
          <pattern name="value_pat" type="int">$jube_pat_int</pattern>
20
          <!-- A combination of a pattern and a parameter -->
21
          <pattern name="dep_pat" type="int" mode="python">$value_pat+$value</pattern>
22
          <!-- This pattern is not available -->
23
          <pattern name="missing_pat" type="int">
24
           pattern_not_available: $jube_pat_int
25
26
          <!-- The combination will fail (create NaN) -->
27
          <pattern name="missing_dep_pat" type="int" mode="python">
28
            $missing_pat*$value
29
          </pattern>
30
31
          <!-- Default value for missing pattern -->
          <pattern name="missing_pat_def" type="int" default="0">
32
           pattern_not_available: $jube_pat_int
33
          </pattern>
34
          <!-- Combination of default value and parameter -->
35
          <pattern name="missing_def_dep_pat" type="int" mode="python">
36
            $missing_pat_def*$value
37
          </pattern>
38
       </patternset>
39
40
        <analyser name="analyse">
41
          <use>pattern_set</use>
42
          <analyse step="operation">
43
            <file>stdout</file>
44
          </analyse>
45
        </analyser>
```

```
47
       <!-- result table creation -->
48
      <result>
        <use>analyse</use>
        51
          <column>value</column>
52
          <column>value_pat</column>
53
          <column>dep_pat</column>
54
          <column>missing_pat</column>
55
          <column>missing_dep_pat</column>
56
          <column>missing_pat_def</column>
57
58
          <column>missing_def_dep_pat</column>
59
         60
      </result>
     </benchmark>
   </jube>
62
```

The input file scripting_pattern.yaml:

```
name: scripting_pattern
   outpath: bench_run
   comment: A scripting_pattern example
   #Configuration
   parameterset:
     name: param_set
     parameter: {name: value, type: int, _: "0,1,2"}
   #Operation
11
   step:
12
     name: operation
13
     use: param_set
     do: echo "$value"
14
15
   #Pattern to extract
16
17
   patternset:
     name: pattern_set
18
     pattern:
19
       #A normal pattern
20
       - {name: value_pat, type: int, _: $jube_pat_int}
21
       #A combination of a pattern and a parameter
22
       - {name: dep_pat, type: int, mode: python, _: $value_pat+$value}
23
       #This pattern is not available
24
       - {name: missing_pat, type: int, _: "pattern_not_available: $jube_pat_int"}
25
       #The combination will fail (create NaN)
26
       - {name: missing_dep_pat, type: int, mode: python, _: $missing_pat*$value}
27
       #Default value for missing pattern
28
       - {name: missing_pat_def, type: int, default: 0, _: "pattern_not_available:
    →$jube_pat_int"}
       #Combination of default value and parameter
       - {name: missing_def_dep_pat, type: int, mode: python, _: $missing_pat_def*
31

$value}

32
   analyser:
33
     name: analyse
34
     use: pattern_set
35
36
     analyse:
       step: operation
37
       file: stdout
38
   #result table creation
```

```
41  result:
42  use: analyse
43  table:
44  name: result
45  style: pretty
46  column: [value,value_pat,dep_pat,missing_pat,missing_dep_pat,missing_pat_def,
    →missing_def_dep_pat]
```

It will create the following output:

```
| value | value_pat | dep_pat | missing_pat | missing_dep_pat | missing_pat_def |_
→missing_def_dep_pat |
  ----|----|--
                 ----|
    0 |
            0 |
                    0 |
                                         nan |
                                                        0 | _
             0 |
    1 |
            1 |
                    2 |
                                         nan |
                                                        0 | _
             0 |
            2 |
                    4 |
    2 |
                               0 |
                                         nan |
             0 |
```

3.4 Statistic pattern values

Normally a pattern should only match a single entry in your result files. But sometimes there are multiple similar entries (e.g. if the benchmark uses some iteration feature).

JUBE will create the statistical values last, min, max, avg, std, cnt and sum automatically. To use these values, the user have to specify the pattern name followed by _<statistic_option>, e.g. pattern_name_last (the pattern_name itself will always be the first match).

An example for multiple matches and the statistic values can be found in examples/statistic.

The input file statistic.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="reduce_example" outpath="bench_run">
       <comment>A result reduce example
       <!-- Regex pattern -->
       <patternset name="pattern">
         <pattern name="number_pat" type="int">$jube_pat_int</pattern>
       </patternset>
10
       <!-- Operation -->
11
       <step name="write_some_numbers">
12
         <do>echo "1 2 3 4 5 6 7 8 9 10"</do> <!-- shell command -->
13
14
       </step>
15
       <!-- Analyse -->
16
       <analyser name="analyse">
17
         <use>pattern</use> <!-- use existing patternset -->
18
         <analyse step="write_some_numbers">
19
           <file>stdout</file> <!-- file which should be scanned -->
20
         </analyse>
21
       </analyser>
22
23
24
       <!-- Create result table -->
       <result>
```

```
<use>analyse</use> <!-- use existing analyser -->
26
        27
          <column>number_pat</column> <!-- first match -->
          <column>number_pat_first</column> <!-- first match -->
          <column>number_pat_last!-- last match -->
30
          <column>number_pat_min</column> <!-- min of all matches -->
31
          <column>number_pat_max</column> <!-- max of all matches -->
32
          <column>number_pat_sum</column> <!-- sum of all matches -->
33
          <column>number_pat_cnt</column> <!-- number of matches -->
34
          <column>number_pat_avg</column> <!-- avg of all matches -->
35
           <column format=".2f">number_pat_std</column> <!-- std of all matches -->
36
37
        38
       </result>
39
     </benchmark>
   </jube>
```

The input file statistic.yaml:

```
name: reduce_example
   outpath: bench_run
   comment: A result reduce example
   #Regex pattern
   patternset:
     name: pattern
     pattern: {name: number_pat, type: int, _: $jube_pat_int}
   #Operation
   step:
11
12
     name: write_some_numbers
     do: echo "1 2 3 4 5 6 7 8 9 10" #shell command
13
14
   #Analvse
15
   analyser:
16
     name: analyse
17
     use: pattern #use existing patternset
18
19
     analyse:
       step: write_some_numbers
20
       file: stdout #file which should be scanned
21
22
   #Create result table
23
   result:
24
     use: analyse #use existing analyser
25
     table:
26
       name: result
27
       style: pretty
28
       column:
29
         - number_pat #first match
         - number_pat_first #first match
31
         - number_pat_last #last match
32
         - number_pat_min #min of all matches
33
          - number_pat_max #max of all matches
34
          - number_pat_sum #sum of all matches
35
          - number_pat_cnt #number of matches
36
          - number_pat_avg #avg of all matches
37
          - {_: number_pat_std, format: .2f} #std of all matches
38
```

It will create the following output:

```
| number_pat | number_pat_last | number_pat_min | number_pat_max | number_pat_sum_

→| number_pat_cnt | number_pat_avg | number_pat_std |
```

3.5 Jobsystem

In most cases you want to submit jobs by *JUBE* to your local jobsystem. You can use the normal file access and substitution system to prepare your jobfile and send it to the jobsystem. *JUBE* also provide some additional features.

The files used for this example can be found inside examples/jobsystem.

The input jobsystem file job.run.in for *Torque/Moab* (you can easily adapt your personal jobscript):

```
#!/bin/bash -x

#MSUB -l nodes=#NODES#:ppn=#PROCS_PER_NODE#

#MSUB -l walltime=#WALLTIME#

#MSUB -e #ERROR_FILEPATH#

#MSUB -o #OUT_FILEPATH#

#MSUB -M #MAIL_ADDRESS#

#MSUB -m #MAIL_MODE#

### start of jobscript

#EXEC#

touch #READY#
```

The JUBE input file jobsystem.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="jobsystem" outpath="bench_run">
       <comment>A jobsystem example
       <!-- benchmark configuration -->
6
       <parameterset name="param_set">
7
         <parameter name="number" type="int">1,2,4</parameter>
8
       </parameterset>
10
       <!-- Job configuration -->
11
       <parameterset name="executeset">
12
         <parameter name="submit_cmd">msub</parameter>
13
         <parameter name="job_file">job.run</parameter>
14
         <parameter name="nodes" type="int">1</parameter>
15
         <parameter name="walltime">00:01:00</parameter>
16
         <parameter name="ppn" type="int">4</parameter>
17
         <parameter name="ready_file">ready</parameter>
18
         <parameter name="mail_mode">abe</parameter>
19
         <parameter name="mail_address"></parameter>
         <parameter name="err_file">stderr</parameter>
21
         <parameter name="out_file">stdout</parameter>
22
         <parameter name="exec">echo $number</parameter>
23
       </parameterset>
24
25
       <!-- Load jobfile -->
26
27
       <fileset name="files">
28
         <copy>${job_file}.in</copy>
       </fileset>
```

```
30
        <!-- Substitute jobfile -->
31
       <substituteset name="sub_job">
32
         <iofile in="${job_file}.in" out="$job_file" />
33
         <sub source="#NODES#" dest="$nodes" />
34
         <sub source="#PROCS_PER_NODE#" dest="$ppn" />
35
         <sub source="#WALLTIME#" dest="$walltime" />
36
         <sub source="#ERROR_FILEPATH#" dest="$err_file" />
37
         <sub source="#OUT_FILEPATH#" dest="$out_file" />
38
         <sub source="#MAIL_ADDRESS#" dest="$mail_address" />
39
         <sub source="#MAIL_MODE#" dest="$mail_mode" />
40
41
         <sub source="#EXEC#" dest="$exec" />
42
          <sub source="#READY#" dest="$ready_file" />
43
       </substituteset>
44
       <!-- Operation -->
45
       <step name="submit" work_dir="$$SCRATCH/jobsystem_bench_${jube_benchmark_id}_$</pre>
46
    →{jube_wp_id}" >
         <use>param_set</use>
47
         <use>executeset</use>
48
         <use>files,sub_job</use>
49
          <do done_file="$ready_file">$submit_cmd $job_file</do> <!-- shell command -->
50
       </step>
51
     </benchmark>
52
   </jube>
```

The JUBE input file jobsystem.yaml:

```
name: jobsystem
   outpath: bench_run
2
   comment: A jobsystem example
   parameterset:
5
     #benchmark configuration
6
     - name: param_set
7
       parameter: {name: number, type: int, _: "1,2,4"} #comma separated integer...
8
    →must be quoted
     #Job configuration
     - name: executeset
10
11
       parameter:
         - {name: submit_cmd, "_": msub}
12
         - {name: job_file, "_": job.run}
13
         - {name: nodes, type: int, "_": 1}
14
         - {name: walltime, "_": "00:01:00"} #: must be quoted
15
         - {name: ppn, type: int, "_": 4}
16
         - {name: ready_file, "_": ready}
17
          - {name: mail_mode, "_": abe}
18
         - {name: mail_address}
19
         - {name: err_file, "_": stderr}
         - {name: out_file, "_": stdout}
21
         - {name: exec, "_": echo $number}
22
23
   #Load jobfile
24
   fileset:
25
     name: files
26
27
     copy: ${job_file}.in
28
   substituteset:
     name: sub_job
30
     iofile: {in: "${job_file}.in", out: $job_file} #attributes with {} must be quoted
31
32
```

(continues on next page)

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```
- {source: "#NODES#", dest: $nodes}
33
       - {source: "#PROCS_PER_NODE#", dest: $ppn}
34
       - {source: "#WALLTIME#", dest: $walltime}
35
       - {source: "#ERROR_FILEPATH#", dest: $err_file}
       - {source: "#OUT_FILEPATH#", dest: $out_file}
37
       - {source: "#MAIL_ADDRESS#", dest: $mail_address}
38
       - {source: "#MAIL_MODE#", dest: $mail_mode}
39
       - {source: "#EXEC#", dest: $exec}
40
       - {source: "#READY#", _: $ready_file } # _ can be used here as well instead of_
41
    →dest (should be used for multiline output)
42
   #Operation
43
   step:
44
45
     name: submit
46
     work_dir: "$$WORK/jobsystem_bench_${jube_benchmark_id}_${jube_wp_id}"
     use: [param_set, executeset, files, sub_job]
47
48
       done_file: $ready_file
49
       _: $submit_cmd $job_file #shell command
50
```

As you can see the jobfile is very general and several parameters will be used for replacement. By using a general jobfile and the substitution mechanism you can control your jobsystem directly out of your *JUBE* input file. \$\$ is used for *Shell* substitutions instead of *JUBE* substitution (see *Environment handling*).

The submit command is a normal Shell command so there are no special JUBE tags to submit a job.

There are two new attributes:

• done_file inside the <do> allows you to set a filename/path to a file which should be used by the jobfile to mark the end of execution. *JUBE* does not know when the job ends. Normally it will return when the *Shell* command was finished. When using a jobsystem the user usually have to wait until the jobfile is executed. If *JUBE* found a <do> containing a done_file attribute *JUBE* will return directly and will not continue automatically until the done_file exists. If you want to check the current status of your running steps and continue the benchmark process if possible you can type:

```
>>> jube continue bench_run
```

This will continue your benchmark execution (bench_run is the benchmarks directory in this example). The position of the done_file is relatively seen towards the work directory.

• work_dir can be used to change the sandbox work directory of a step. In normal cases JUBE checks that every work directory gets a unique name. When changing the directory the user must select a unique name by his own. For example he can use <code>\$jube_benchmark_id</code> and <code>\$jube_wp_id</code>, which are JUBE internal parameters and will be expanded to the current benchmark and workpackage ids. Files and directories out of a given <code>fileset</code> will be copied into the new work directory. Other automatic links, like the dependency links, will not be created!

You will see this Output after running the benchmark:

and this output after running the continue command (after the jobs where executed):

You have to run continue multiple times if not all done_file were written when running continue for the first time.

3.6 Include external data

As you have seen in the example before a benchmark can become very long. To structure your benchmark you can use multiple files and reuse existing sets. There are three different include features available.

The files used for this example can be found inside examples/include.

The include file include_data.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
     <parameterset name="param_set">
       <parameter name="number" type="int">1,2,4</parameter>
     </parameterset>
     <parameterset name="param_set2">
       <parameter name="text">Hello</parameter>
     </parameterset>
10
     <dos>
11
       <do>echo Test</do>
12
       <do>echo $number</do>
13
14
     </dos>
15
   </jube>
```

The include file include_data.yaml:

```
parameterset:
    - name: param_set
    parameter: {name: number, type: int, _: "1,2,4"}
    - name: param_set2
    parameter: {name: text, _: Hello}

dos:
    - echo Test
    - echo $number
```

All files which contain data to be included must use the *XML*-format. The include files can have a user specific structure (there can be no valid *JUBE* tags like <dos>), but the structure must be allowed by the searching mechanism (see below). The resulting file must have a valid *JUBE* structure.

The main file main.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="include" outpath="bench_run">
3
       <comment>A include example
4
5
       <!-- use parameterset out of an external file and add a additional parameter --
6
       <parameterset name="param_set" init_with="include_data.xml">
         <parameter name="foo">bar</parameter>
       </parameterset>
10
       <!-- Operation -->
11
       <step name="say_hello">
12
         <use>param_set</use> <!-- use existing parameterset -->
13
         <use from="include_data.xml">param_set2</use> <!-- out of an external file --</pre>
14
         <do>echo $foo</do> <!-- shell command -->
15
         <include from="include_data.xml" path="dos/do" /> <!-- include all available_</pre>
```

The main file main.yaml:

```
name: include
   outpath: bench_run
   comment: A include example
   #use parameterset out of an external file and add a additional parameter
   parameterset:
     name: param set
     init_with: include_data.yaml
     parameter: {name: foo, _: bar}
10
11
   #Operation
12
   step:
13
     name: say_hello
14
     use:
      - param_set #use existing parameterset
15
      - from: include_data.yaml
16
         _: param_set2 #out of an external file
17
18
       - echo $foo
19
       - !include include_data.yaml:["dos"] #include all available tag
```

In these file there are three different include types:

The init_with can be used inside any set definition. Inside the given file the search mechanism will search for the same set (same type, same name), will parse its structure (this must be JUBE valid) and copy the content to main.xml. Inside main.xml you can add additional values or overwrite existing ones. If your include-set uses a different name inside your include file you can use init_with="filename.xml:old_name". It is possible to mix YAML based include files with XML files and vice versa.

The second method is the <use from="...">. This is mostly the same like the init_with structure, but in this case you are not able to add or overwrite some values. The external set will be used directly. There is no set-type inside the <use>>, because of that, the set's name must be unique inside the include-file. The remote file can use the YAML or the XML format.

The last method is the most generic include. The include mechanic is the only element in *JUBE* which works slightly different in *YAML* and *XML* based files.

In XML based files by using <include /> you can copy any XML-nodes you want to your main-XML file. The included file can provide tags which are not JUBE-conform but it must be a valid XML-file (e.g. only one root node allowed). The resulting main configuration file must be completely JUBE valid. The path is optional and can be used to select a specific node set (otherwise the root-node itself will be included). The <include /> will copy all parts without any changes. The other include types will update path names, which were relative to the include-file position.

In *YAML* based files the prefix! include is used followed by the file name. The file must be a *YAML* file, which will be opened and parsed. The second block: ["dos"] can be used to select any subset of data of the full dictionary, any Python syntax is allowed for this selection. Finally it is possible to also specify a third block which allows full Python list comprehensions. _ is the match of the selection before, e.g.: !include include_data.yaml: ["dos"]: [i for i in _ if "Test" in i]. In contrast to the *XML* based include it isn't possible to mix lists or dictionaries out of different files, each key can only handle a single include.

To run the benchmark you can use the normal command:

```
>>> jube run main.xml
```

It will search for the files to include inside four different positions, in the following order:

• inside a directory given over the command line interface:

```
>>> jube run --include-path some_path another_path -- main.xml
```

• inside any path given by an <include-path>-tag:

```
<
```

• inside any path given with the JUBE_INCLUDE_PATH environment variable (see Configuration):

```
>>> export JUBE_INCLUDE_PATH=some_path:another_path
```

• inside the same directory of your main.xml

JUBE stops searching as soon as it finds the file to include, or gives an error if the file is not found.

3.7 Tagging

Tagging is an easy way to hide selectable parts of your input file.

The files used for this example can be found inside examples/tagging.

The input file tagging.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
     <benchmark name="tagging" outpath="bench_run">
       <comment>Tags as logical combination
       <!-- Configuration -->
       <parameterset name="param_set">
         <parameter name="hello_str" tag="!deu+eng">Hello</parameter>
         <parameter name="hello_str" tag="deu|!eng">Hallo</parameter>
         <parameter name="world_str" tag="eng">World</parameter>
10
       </parameterset>
11
12
       <!-- Operation -->
13
       <step name="say_hello">
14
         <use>param_set</use> <!-- use existing parameterset -->
15
         <do>echo '$hello_str $world_str'</do> <!-- shell command -->
16
       </step>
17
     </benchmark>
18
   </jube>
19
```

The input file tagging.yaml:

```
name: tagging
outpath: bench_run
comment: Tags as logical combination

#Configuration
parameterset:
name: param_set
parameter:
```

(continues on next page)

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```
- {name: hello_str, tag: "!deu+eng", _: Hello}
       - {name: hello_str, tag: deu|!eng, _: Hallo}
10
       - {name: world_str, tag: eng, _: World}
11
12
   #Operation
13
   step:
14
     name: say_hello
15
     use: param_set #use existing parameterset
16
     do: echo '$hello_str $world_str' #shell command
17
```

When running this example:

```
>>> jube run tagging.xml
```

All <tags> which contain a special tag="..." attribute will be hidden if the tag results to false. !deu stands for not deu. To connect the tags | can be used as the oprator OR and + for the operator AND. Also brackets are allowed.

The result (if no tag is set on the commandline) inside the stdout file will be

```
Hallo $world_str
```

because !deu+eng and eng will be false and there is no other input available for \$world_str.deu|!eng will be true.

When running the same example using a specific tag:

```
>>> jube run tagging.xml --tag eng
```

the result inside the stdout file will be

```
Hello World
```

A tag which results to false will trigger to complety ignore the corresponding <tag>! If there is no alternative this can produce a wrong execution behaviour!

Also a list of tags, separated by spaces, can be provided on the commandline.

The tag attribute can be used inside every <tag> inside the input file (except the <jube>).

3.8 Platform independent benchmarking

If you want to create platform independent benchmarks you can use the include features inside of JUBE.

All platform related sets must be declared in an includable file e.g. platform.xml. There can be multiple platform.xml in different directories to allow different platforms. By changing the include-path the benchmark changes its platform specific data.

An example benchmark structure is based on three include files:

- The main benchmark include file which contain all benchmark specific but platform independent data
- A mostly generic platform include file which contain benchmark independent but platform specific data (this can be created once and placed somewhere central on the system, it can be easily accessed using the JUBE_INCLUDE_PATH environment variable.
- A platform specific and benchmark specific include file which must be placed in a unique directory to allow inlcude-path usage

Inside the platform directory you will find some example benchmark independent platform configuration files for the supercomputers at Forschungszentrum Jülich.

To avoid writing long include-paths every time you run a platform independent benchmark, you can store the include-path inside your input file. This can be mixed using the tagging-feature:

```
</path tag="plat1">some path</path>

<pre
```

Now you can run your benchmark using:

```
>>> jube run filename.xml --tag plat1
```

3.9 Multiple benchmarks

Often you only have one benchmark inside your input file. But it is also possible to store multiple benchmarks inside the same input file:

```
- name: a

# data for benchmark a

- name: b

# data for benchmark b
```

All benchmarks can use the same global (as a child of <jube>) declared sets. Often it might be better to use an include feature instead. *JUBE* will run every benchmark in the given order. Every benchmark gets a unique benchmark id.

To select only one benchmark you can use:

```
>>> jube run filename.xml --only-bench a
```

or:

```
>>> jube run filename.xml --not-bench b
```

This information can also be stored inside the input file:

3.10 Shared operations

Sometimes you want to communicate between the different workpackages of a single step or you want a single operation to run only once for all workpackages. Here you can use shared steps.

The files used for this example can be found inside examples/shared.

The input file shared.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="shared" outpath="bench_run">
       <comment>A shared folder example
4
       <!-- Configuration -->
       <parameterset name="param_set">
         <parameter name="number" type="int">1,2,4</parameter>
       </parameterset>
10
11
       <!-- Operation -->
12
       <step name="a_step" shared="shared">
13
         <use>param_set</use>
         <!-- shell command will run three times -->
14
         <do>echo $jube_wp_id >> shared/all_ids</do>
15
         <!-- shell command will run one time -->
16
         <do shared="true">cat all_ids</do>
17
18
       </step>
     </benchmark>
19
   </jube>
20
```

The input file shared.yaml:

```
name: shared
   outpath: bench_run
   comment: A shared folder example
   #Configuration
   parameterset:
     name: param_set
     parameter: {name: number, type: int, _: "1,2,4"}
10
   #Operation
11
   step:
     name: a_step
12
     shared: shared
13
     use: param_set
14
15
       - echo $jube_wp_id >> shared/all_ids #shell command will run three times
16
         {shared: true, _: cat all_ids} #shell command will run one times
```

The step must be marked using the shared attribute. The name, given inside this attribute, will be the name of a symbolic link, which will be created inside every single sandbox work directory pointing to a single shared folder. Every Workpackage can access this folder by using its own link. In this example every workpackage will write its own id into a shared file (\$jube_wp_id is an internal variable, more of these you will find here).

To mark an operation to be a shared operation shared="true" inside the <do> must be used. The shared operation will start after all workpackages reached its execution position. The work directory for the shared operation is the shared folder itself.

You will get the following directory structure:

```
+- 000000
                            # the benchmark id
      +- configuration.xml # the stored benchmark configuration
      +- workpackages.xml # workpackage information
      +- 000000_a_step
                           # the first workpackage
         +- done
                            # workpackage finished marker
                            # user sandbox folder
         +- work
10
11
            +- stderr
                            # standard error messages of used shell commands
12
            +- stdout
                            # standard output of used shell commands
13
            +- shared
                            # symbolic link pointing to shared folder
14
      +- 000001_a_step
                            # workpackage information
15
16
      +- 000002_a_step
                            # workpackage information
                            # the shared folder
17
      +- a_step_shared
18
         +- stdout
                            # standard output of used shell commands
19
         +- stderr
                            # standard error messages of used shell commands
20
         +- all_ids
                            # benchmark specific generated file
21
```

3.11 Environment handling

Shell environment handling can be very important to configure paths or parameter of your program.

The files used for this example can be found inside examples/environment.

The input file environment.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
     <benchmark name="environment" outpath="bench_run">
       <comment>An environment handling example
       <!-- Configuration -->
6
       <parameterset name="param_set">
         <parameter name="EXPORT_ME" export="true">VALUE</parameter>
       </parameterset>
10
       <!-- Operations -->
11
       <step name="first_step" export="true">
12
         <do>export SHELL_VAR=Hello</do> <!-- export a Shell var -->
13
         <do>echo "$$SHELL_VAR world"</do><!-- use exported Shell var -->
14
       </step>
15
16
       <!-- Create a dependency between both steps -->
17
       <step name="second_step" depend="first_step">
18
         <use>param_set</use>
19
20
         <do>echo $$EXPORT_ME</do>
         <do>echo "$$$HELL_VAR again"</do> <!-- use exported Shell var out of_</pre>
21
    →privious step -->
       </step>
22
     </benchmark>
23
   </jube>
24
```

The input file environment.yaml:

```
name: environment
outpath: bench_run
comment: An environment handling example
```

```
#Configuration
   parameterset:
     name: param_set
     parameter: {name: EXPORT_ME, export: true, _: VALUE}
10
   step:
     #Operation
11
     - name: first_step
12
       export: true
13
14
         - export SHELL_VAR=Hello #export a Shell var
15
         - echo "$$$HELL_VAR world" #use exported Shell var
16
17
18
      #Create a dependency between both steps
19
     - name: second_step
       depend: first_step
20
       use: param_set
21
       do:
22
          - echo $$EXPORT_ME
23
         - echo "$$$HELL_VAR again" #use exported Shell var out of privious step
```

In normal cases all <do> within one <step> shares the same environment. All **exported** variables of one <do> will be available inside the next <do> within the same <step>.

By using export="true" inside of a <parameter> you can export additional variables to your *Shell* environment. Be aware that this example uses \$\$ to explicitly use *Shell* substitution instead of *JUBE* substitution.

You can also export the complete environment of a step to a dependent step by using export="true" inside of <step>.

3.12 Parameter dependencies

Sometimes you need parameters which are based on other parameters or only a specific parameter combination makes sense and other combinations are useless or wrong. For this there are several techniques inside of *JUBE* to create such a more complex workflow.

The files used for this example can be found inside examples/parameter_dependencies.

The input file parameter_dependencies.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="parameter_dependencies" outpath="bench_run">
       <comment>A parameter_dependencies example
       <!-- Configuration -->
       <parameterset name="param_set">
         <parameter name="index" type="int">0,1</parameter>
         <parameter name="text" mode="python">["hello", "world"][$index]
       </parameterset>
10
11
       <parameterset name="depend_param_set0">
12
         <parameter name="number" type="int">3,5</parameter>
13
       </parameterset>
14
15
       <parameterset name="depend_param_set1">
16
         <parameter name="number" type="int">1,2,4</parameter>
17
       </parameterset>
18
19
```

```
<!-- Operation -->
20
       <step name="operation">
21
         <use>param_set</use> <!-- use basic parameterset -->
22
          <use>depend_param_set$index</use> <!-- use dependent parameterset -->
23
          <use from="include_file.xml:depend_param_set0:depend_param_set1">
24
25
            depend_param_set$index
          </use>
26
          <do>echo "$text $number $number2"</do>
27
       </step>
28
     </benchmark>
29
   </jube>
30
```

The input file parameter_dependencies.yaml:

```
name: parameter_dependencies
   outpath: bench_run
   comment: A parameter_dependencies example
   #Configuration
   parameterset:
     - name: param_set
       parameter:
         - {name: index, type: int, _: "0,1"} #comma separated integer must be in_
   -- quotations
         - {name: text, mode: python, _: '["hello", "world"][$index]'} #attributes_
10
   →with " and [] must be in quotations
     - name: depend_param_set0
11
      parameter: {name: number, type: int, _: "3,5"} #comma separated integer must...
12
   →be in quotations
13
     - name: depend_param_set1
       parameter: {name: number, type: int, _: "1,2,4"} #comma separated integer_
14
   →must be in quotations
15
   #Operation
16
   step:
17
     name: operation
18
19
       - param_set #use basic parameterset
20
       - depend_param_set$index #use dependent parameterset
21
       - {from: 'include_file.yaml:depend_param_set0:depend_param_set1', _: depend_
22
   →param_set$index}
     do: echo "$text $number $number2"
23
```

The include file include file.xml:

The include file include_file.yaml:

```
- name: depend_param_set1
parameter: {name: number2, type: int, _: 20}
```

The easiest way to handle dependencies is to define an index-parameter which can be used in other scripting parameters to combine all dependent parameter combinations.

Also complete sets can be marked as dependent towards a specific parameter by using this parameter in the <use>-tag. When using parametersets out of an other file the correct set-name must be given within the from attribute, because these sets will be loaded in a pre-processing step before the corresponding parameter will be evaluated. Also sets out of different files can be combined within the same <use> by using the file1:set1, file2:set2 syntax. The sets names must be unique.

3.13 Parameter update

Once a parameter is specified and evaluated the first time, its value will not change. Sometimes this behaviour can produce the wrong behaviour:

```
<parameter name="foo">$jube_wp_id</parameter>
```

In this example foo should hold the \$jube_wp_id. If you have two steps, where one step depends on the other one foo will be available in both, but it will only be evaluated in the first one.

There is a simple workaround to change the update behaviour of a parameter by using the attribute update_mode:

- update_mode="never" No update (default behaviour)
- update_mode="use" Re-evaluate the parameter if the parameterset is explicitly used
- update_mode="step" Re-evaluate the parameter for each new step
- update_mode="cycle" Re-evaluate the parameter for each new cycleloop, but not at the begin of a new step
- update_mode="always" Combine step and cycle

Within a cycle loop no new workpackages can be created. Templates will be reevaluated, but they can not increase the number of existing workpackages within a cycle.

Within the result generation, the parameter value, which is presented in the result table is the value of the selected analysed step. If another parameter representation is needed as well, all other steps can be reached by using parameter_name>_<step_name>.

The files used for this example can be found inside examples/parameter_update.

The input file parameter_update.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="parameter_updates" outpath="bench_run">
       <comment>A parameter_update example
4
       <!-- Configuration -->
6
       <parameterset name="foo">
         <parameter name="bar_never" mode="text" update_mode="never">
           iter_never: $jube_wp_id
         </parameter>
10
         <parameter name="bar_use" mode="text" update_mode="use">
11
           iter_use: $jube_wp_id
12
         </parameter>
13
         <parameter name="bar_step" mode="text" update_mode="step">
14
           iter_step: $jube_wp_id
15
```

```
</parameter>
16
        </parameterset>
17
        <!-- Operation -->
        <step name="step1">
20
          <use>foo</use>
21
          <do>echo $bar_never</do>
22
          <do>echo $bar_use</do>
23
          <do>echo $bar_step</do>
24
        </step>
25
26
27
        <step name="step2" depend="step1">
28
          <use>foo</use>
29
          <do>echo $bar_never</do>
30
          <do>echo $bar_use</do>
          <do>echo $bar_step</do>
31
32
        </step>
33
        <step name="step3" depend="step2">
34
          <do>echo $bar_never</do>
35
          <do>echo $bar_use</do>
36
          <do>echo $bar_step</do>
37
        </step>
38
      </benchmark>
   </jube>
```

The input file parameter_update.yaml:

```
name: parameter_updates
2
   outpath: bench_run
3
   comment: A parameter_update example
   #Configuration
5
   parameterset:
6
     name: foo
7
     parameter:
8
        - {name: bar_never, mode: text, update_mode: never, _: "iter_never: $jube_wp_id
        - {name: bar_use, mode: text, update_mode: use, _: "iter_use: $jube_wp_id"}
10
        - {name: bar_step, mode: text, update_mode: step, _: "iter_step: $jube_wp_id"}
11
12
   #Operation
13
   step:
14
     - name: step1
15
       use: foo
16
17
         - echo $bar_never
18
         - echo $bar_use
19
20
          - echo $bar_step
21
     - name: step2
       depend: step1
22
       use: foo
23
        do:
24
          - echo $bar_never
25
          - echo $bar use
26
27
          - echo $bar_step
      - name: step3
28
        depend: step2
29
        do:
30
          - echo $bar_never
31
          - echo $bar_use
32
```

```
- echo $bar_step
```

The use and influence of the three update modes update_mode="never", update_mode="use" and update_mode="step" is shown here. Keep in mind, that the steps have to be dependent from each other leading to identical outputs otherwise.

3.14 Step iteration

Especially in the context of benchmarking, an application should be executed multiple times to generate some meaningful statistical values. The handling of statistical values is described in *Statistic pattern values*. This allows you to aggregate multiple result lines if your application automatically support to run multiple times.

In addition there is also an iteration feature within JUBE to run a specific step and its parametrisation multiple times.

The files used for this example can be found inside examples/iterations.

The input file iterations.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
     <benchmark name="iterations" outpath="bench_run">
       <comment>A Iteration example
       <!-- Configuration -->
       <parameterset name="param_set">
         <parameter name="foo" type="int">1,2,4</parameter>
         <parameter name="bar" mode="text" update_mode="step">$foo iter:$jube_wp_
    →iteration/parameter>
       </parameterset>
10
11
       <step name="first_step" iterations="2">
12
13
         <use>param_set</use> <!-- use existing parameterset -->
         <do>echo $bar</do> <!-- shell command -->
       </step>
16
       <step name="second_step" depend="first_step" iterations="2">
17
         <do>echo $bar</do> <!-- shell command -->
18
       </step>
19
20
       <!-- analyse without reduce -->
21
       <analyser name="analyse_no_reduce" reduce="false">
22
         <analyse step="second_step" />
23
       </analyser>
24
25
       <!-- Analyse with reduce -->
26
       <analyser name="analyse" reduce="true">
27
         <analyse step="second_step" />
28
       </analyser>
29
30
       <result>
31
         <use>analyse</use>
32
33
         <use>analyse_no_reduce</use>
         34
           <column>jube_res_analyser</column>
35
           <column>jube_wp_id_first_step</column>
36
           <column>jube_wp_id</column>
37
           <column>jube_wp_iteration_first_step</column>
38
           <column>jube_wp_iteration</column>
39
           <column>foo</column>
40
```

The input file iterations.yaml:

```
name: iterations
2
   outpath: bench_run
   comment: A Iteration example
   #Configuration
   parameterset:
6
     name: param_set
     parameter:
8
        - {name: foo, type: int, _: "1,2,4"}
        - {name: bar, update_mode: step, _: '$foo iter:$jube_wp_iteration'}
10
11
12
   step:
     - name: first_step
13
        iterations: 2
14
        use: param_set #use existing parameterset
15
        do: echo $bar #shell command
16
      - name: second_step
17
        depend: first_step
18
        iterations: 2
19
        do: echo $bar #shell command
20
21
   analyser:
22
23
     #analyse without reduce
24
      - name: analyse_no_reduce
        reduce: false
25
        analyse:
26
          step: second_step
27
      #analyse with reduce
28
29
      - name: analyse
        reduce: true
30
        analyse:
31
          step: second_step
32
33
   result:
34
     use: [analyse, analyse_no_reduce]
35
     table:
36
       name: result
37
        style: pretty
38
        column:
39
          - jube_res_analyser
40
          - jube_wp_id_first_step
41
          - jube_wp_id
42
          - jube_wp_iteration_first_step
43
44
          - jube_wp_iteration
          - foo
45
```

In this example, both steps 1 and 2 are executed 2 times for each parameter and dependency configuration. Because of the given parameter, step 1 is executed 6 times in total (3 parameter combinations x 2). Step 2 is executed 12 times (6 from the dependent step x 2). Each run will be executed in the normal way using its individual sandbox folder.

\$jube_wp_iteration holds the individual iteration id. The update_mode is needed here to reevaluate the parameter bar in step 2.

In the analyser reduce=true or reduce=false can be enabled, to allow you to see all individual results or

to aggregate all results of the same parameter combination. for the given step. If reduce=true is enabled (the default behaviour) the output of the individual runs, which uses the same parametrisation, are treated like a big continuous file before applying the statistical patterns.

```
| jube_res_analyser | jube_wp_id_first_step | jube_wp_id | jube_wp_iteration_first_
   →step | jube_wp_iteration | foo |
   ⇔-----|-----|
                                        0 |
   | analyse_no_reduce |
                                                    6 |
                        0 | 1 |
   → 0 |
                                        0 |
                                                    7 |
   | analyse_no_reduce |
      0 |
                         1 | 1 |
                                        1 |
                                                    8 |
   | analyse_no_reduce |
                         2 | 1 |
      1 |
                                        1 |
   | analyse_no_reduce |
      1 |
                         3 |
                              1 |
   | analyse_no_reduce |
                                        2 |
                                                   10 |
   → 0 |
                         0 |
                              2 |
   | analyse_no_reduce |
                                        2 |
                                                   11 |
   → 0 |
                         1 |
                              2 |
9
   | analyse_no_reduce |
                                        3 |
                                                   12 |
   2 |
                              2 |
   | analyse_no_reduce |
                                        3 |
                                                   13 |
10
   3 |
                              2 |
   | analyse_no_reduce |
                                        4 |
                                                   14 |
11
   0 |
                              4 |
   | analyse_no_reduce |
                                                   15 |
12
   → 0 |
                         1 |
                              4 |
   | analyse_no_reduce |
                                        5 |
                                                   16 |
13
   2 |
                              4 |
   | analyse_no_reduce |
                                        5 |
                                                   17 I
14
                         3 |
       1 |
                              4 |
             analyse |
                                        5 |
                                                   16 |
15
       1 |
                         2 |
                              4 |
             analyse |
                                        0 |
                                                   7 |
16
       0 |
                         1 |
                              1 |
             analyse |
                                        1 |
                                                    8 |
17
       1 |
                         2 |
                              1 |
             analyse |
                                        2 |
                                                   10 |
       0 |
                         0 |
                              2 |
                                                   12 |
                                        3 |
19
             analyse |
                         2 |
                              2 |
       1 |
                                        4 |
                                                   15 |
             analyse |
20
       0 |
                         1 |
                              4 |
```

3.15 Step cycle

Instead of having a new workpackage you can also redo the <do> commands inside a step using the cycle-feature. In contrast to the iterations, all executions for the cycle feature take place inside the same folder.

The files used for this example can be found inside examples/cycle.

The input file cycle.xml:

```
</pr
```

```
// do break_file="done">echo $jube_wp_cycle</do>
/do active="$jube_wp_cycle==2">touch done</do>
// step>
// benchmark>
// jube>
// jube>
// constant in the control of the control o
```

The cycles attribute allows to repeat all <do> commands within a step multiple times. The break_file can be used to cancel the loop and all following commands in the current cycle (the command itself is still executed). In the given example the output will be:

```
0
1
2
3
```

In contrast to the iterations, all executions for the cycle feature take place inside of the same folder.

3.16 Parallel workpackages

In a standard jube run a queue is filled with workpackages and then processed in serial. To enable parallel execution of independent workpackages, which belong to the expansions of a step, the argument procs of <step> can be used.

The files used for this example can be found inside examples/parallel_workpackages. The input file parallel_workpackages.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
2
   <jube>
     <benchmark name="parallel_workpackages" outpath="bench_run">
       <comment>A parallel workpackages demo</comment>
       <parameterset name="param_set">
         <parameter name="i" type="int" mode="python">",".join([ str(i) for i in_
   →range(0,10)])/parameter>
       </parameterset>
       <step name="parallel_execution" suffix="${i}" procs="4">
10
         <use>param_set</use>
11
         <do>echo "${i}"</do>
12
         <do>N=1000000; a=1; for (( k = 0; k < $N; ++k)); do a=$(( 2*k + 1 +
13
   →$a )) ; done</do>
14
       </step>
15
     </benchmark>
   </jube>
16
```

```
name: parallel_workpackages
outpath: bench_run
comment: A parallel workpackages demo

parameterset:
name: param_set
parameter: {name: i, type: int, mode: python, _: "\",\".join([ str(i) for i in_ range(0,10)])"}
step:
name: parallel_execution
suffix: ${i}
procs: 4
```

```
use: param_set

do:
    - "echo \"${i}\""
    - "N=1000000; a=1; for (( k = 0; k < $N; ++k)); do a=$(( 2*k + 1 + $a)); ...

    →done"
```

In the example above the expansion of the parameter i will lead to the creation of 10 workpackages of the step parallel_execution. Due to the given argument procs="4" JUBE will start 4 worker processes which will distribute the execution of the workpackages among themselves. N within the JUBE script represents the number of computation iterations to simulate a computational workload at hand. The parameters N, procs and the upper bound of range within this prototypical example can be alternated to study runtime, memory usage and load of CPUs.

Important hints:

- <do shared="true"> is not supported if procs is set for the corresponding step.
- If <step shared="..."> is set, then the user is responsible to avoid data races within the shared directory.
- Switching to an alternative work_dir for a step can also lead to data races if all expansions of the step access the same work_dir. Recommendation: Don't use a shared work_dir in combination with procs.
- This feature is implemented based on the Python package multiprocessing and doesn't support internode communication. That's why the parallelisation is limited to a single shared memory compute node.
- Be considerate when working on a multi-user system with shared resources. The parallel feature of JUBE can easily exploit a whole compute node.
- Parallel execution of a JUBE script can lead to much higher memory demand compared to serial execution with procs=1. In this case it is advised to reduce procs leading to reduced memory usage.

3.17 Result database

Results can also be stored into a database to simplify result management.

The files used for this example can be found inside examples/result_database.

The input file result_database.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="result_database" outpath="bench_run">
       <comment>result database creation
       <parameterset name="param_set">
         <parameter name="number" type="int">1,2,4</parameter>
       </parameterset>
       <patternset name="pattern">
10
         <pattern name="number_pat" type="int">Number: $jube_pat_int</pattern>
11
       </patternset>
12
13
       <step name="write_number">
         <use>param_set</use>
15
         <do>echo "Number: $number"</do>
16
       </step>
17
18
       <analyser name="analyse">
19
         <use>pattern</use>
20
         <analyse step="write_number">
21
```

```
<file>stdout</file>
22
          </analyse>
23
        </analyser>
24
25
        <result>
26
          <use>analyse</use>
27
          <!-- creating a database containing the columns "number" and "number_pat" -->
28
          <!-- one table of the name "results" is created within the database -->
29
          <!-- a database file "result_database.dat" is created in the current working_
30
    →directory -->
          <database name="results" file="result_database.dat" primekeys="number, number_</pre>
31
    ⇔pat">
            <key>number</key>
32
33
            <key>number_pat
34
          </database>
        </result>
35
     </benchmark>
36
   </jube>
37
```

The input file result_database.yaml:

```
name: result_database
   outpath: bench_run
   comment: result database creation
   parameterset:
     name: param_set
     parameter: {name: number, type: int, _: "1,2,4"}
   patternset:
10
     name: pattern
     pattern: {name: number_pat, type: int, _: "Number: $jube_pat_int"}
11
12
   step:
13
     name: write_number
14
     use: param_set
15
     do: "echo \"Number: $number\""
16
17
   analyser:
18
19
     name: analyse
     use: pattern
20
     analyse:
21
       step: write_number
22
       file: stdout
23
24
   result:
25
     use: analyse
26
     database:
27
       # creating a database containing the columns "number" and "number_pat"
28
        # one table of the name "results" is created within the database
29
        # a database file "result_database.dat" is created in the current working_
30
    →directory
       name: results
31
       file: result_database.dat
32
       primekeys: "number, number_pat"
33
       key:
34
35
        - number
       - number_pat
```

The default database will be located as follows and has the database tag name, which is here results, as root name concatenated with the appendix .dat:

3.17. Result database 41

```
bench_run

| bench_run

| color="block" |
```

The database tag takes the argument name. name is also the name of the table created within a database. If sqlite3 is installed the contents of the database can be shown with the following command line.

The argument file states the full path of a second copy of the database file. The path can be stated relative or absolute. In this case the database file result_database.dat is created within the current working directory in which jube result was invoked.

Invocating jube result a second time updates the database given by the file parameter. Without the parameter primekeys three additional lines to the results table would have been added which are completely identical to the previous three lines. Adding the argument primekeys ensures that only if the column values stated within primekeys are not exactly the same in the database table, a new line is added to the database table. In this example no new lines are added. All the primekeys also need to be stated as key. Updating the primekeys is not supported.

The key tag adds columns to the database table having the same type as the corresponding parameter or pattern. Information of columns of the database table results can be shown as follows.

To have a look into a database within a python script the python modules sqalchemy or pandas can be used.

3.18 Creating a do log

To increase reproducibility of the do statements within a workpackage of a step and to archive the environment during execution, a do log can be printed. A do log tries to mimic an executable script recreating the environment at execution time. The files used for this example can be found inside examples/do_log.

The input file do_log.xml:

```
// cyparameterset>

// step name="execute" shared="shared" do_log_file="do_log">
// use>param_set</use>
// cyparam_set
// cyparameterset

//
```

The input file do_log.yaml:

```
name: do_log_example
     outpath: bench_run
2
     parameterset:
       - name: "param_set"
         parameter:
            - {name: "number", _: "1,2,3,4,5"}
     step:
       name: execute
10
11
         - param_set
12
       do_log_file: "do_log"
13
       shared: "shared"
14
15
         - cp ../../../loreipsum${number} shared
16
         - {shared: "true", _: "grep -r -l \"Hidden!\" loreipsum*"}
17
```

In this example a hidden string is searched for within 5 files and the name of the file containing the hidden string is printed.

For the initial execution of this example within bench_run/000000/00000[0-4]_execute each can be found a do_log file. These files can be executed manually by prefixing it with /bin/sh. The scripts will reproduce the environment at execution time, the execution and the result output. Keep in mind that the shared grep will be executed by the benchmark with id 4 only.

3.19 The duplicate option

To simplify advanced tagging and parameter concatenation the duplicate option within parametersets or parameters can be stated.

The input file duplicate.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
     <benchmark name="parameter_duplicate_example" outpath="bench_run">
       <comment>parameter duplicate example</comment>
       <parameterset name="options" duplicate="concat">
         <parameter name="iterations"</pre>
                                                    >1</parameter>
         <parameter name="iterations" tag="few" >2,3,4</parameter>
         <parameter name="iterations" tag="many">20,30,40</parameter>
       </parameterset>
10
11
       <parameterset name="result">
12
         <parameter name="sum" mode="python">int(${iterations}*(${iterations}+1)/2)
     parameter>
                                                                            (continues on next page)
```

The input file duplicate.yaml:

```
name: parameter_duplicate_example
   outpath: bench_run
2
   comment: parameter duplicate example
   parameterset:
6
     - name: options
       duplicate: concat
       parameter:
                                           _: "1"}
         - {name: iterations,
         - {name: iterations, tag: few, _: "2,3,4"}
10
         - {name: iterations, tag: many, _: "20,30,40"}
11
     - name: result
12
       parameter:
13
       - {name: sum, mode: "python", _: "int(${iterations}*(${iterations}+1)/2)"}
14
15
   step:
16
     name: perform_iterations
17
     use: "options, result"
18
     do: "echo $sum"
19
```

In this example the duplicate option with the value concat is stated for a parameterset. This leads to a concatenation of parameter values of the same name. In combination with the tagging option for parameters the user can specify which options are included into the parameters. If the user states the tags few and many the parameter iterations takes the values 1, 2, 3, 4, 20, 30, 40.

The default option of duplicate for parametersets is replace which leads to a replacing of parameters if they are mentioned more than once. A third option for the duplicate option for parametersets is error. In this case the execution is aborted if a parameter is defined more than once.

The option duplicate can also be stated for parameters. In this case the parameters duplicate option is prioritized over the parametersets one. The possible values for parameters duplicate option are none, replace, concat and error. none is the default value and leads to the duplicate option being ignored for this parameter such that the parametersets duplicate option is taking precedence. The other three options have the same effect as in the parameterset.

3.20 The prepare option

In case of compilation-execution workflows one step can be defined to compile a piece of software while another step is executing the compiled binary. Both steps can be combined through the depend option of the step tag. If there are a lot of compilations which take a lot of time for each iteration it is reasonable to reduce the amount of compilations dependent on the executions. The depend option is not suited to achieve this goal. Therefore, there is the prepare option for a step tag.

The prepare option defines a list of steps which are prepared by the current preparation step. If at least one of the prepared steps is available the current preparation step is executed. Otherwise, it is not executed and no errors are thrown unlike in the case of the depend option.

The input file step_prepare.xml:

```
<?xml version="1.0" encoding="UTF-8"?>
   <jube>
2
     <benchmark name="step_prepare_example" outpath="bench_run">
3
       <comment>A step prepare example
       <step name="prepare_step" prepare="execution_step">
6
         <do>python3 --version || exit 1</do>
       </step>
8
       <step name="execution_step" tag="execute">
10
         <do>python3 -c 'import math; print(math.factorial(10))'</do>
11
       </step>
12
13
     </benchmark>
   </jube>
```

The input file step_prepare.yaml:

In this example, the step prepare_step is only executed if the tag execute for the step execution_step is passed to the jube execution. Otherwise, the prepare_step is not executed.

Defining a prepare relationship between to steps is implicitly leading to a reverse depend relationship, such that the depend option is not explicitly needed. Therefore, it is guaranteed that the preparation step is executed before the prepared step.

FREQUENTLY ASKED QUESTIONS

4.1 Parameter groups

Within JUBE you can define parameter groups to allow only specific parameter combinations.

E.g. you have two parameters:

```
<parameter name="foo">10,100</parameter>
<parameter name="bar">20,200</parameter>
```

```
parameter:
   - { name: foo, _: '10,100' }
   - { name: bar, _: '20,200' }
```

Without any additional change, *JUBE* will run four paramater combinations (foo=10,bar=20,foo=100,bar=20,foo=100,bar=200,foo=100,bar=200). But maybe within your configuration only foo=10,bar=20 and foo=100,bar=200 make sense. For this you can use the parameter dependencies feature and small *Python* snippets (*Parameter dependencies*) to split the four combinations into two groups, by using a dummy index value:

```
<parameter name="i">o,1</parameter>
<parameter name="foo" mode="python">[10,100][$i]</parameter>
<parameter name="bar" mode="python">[20,200][$i]</parameter>
```

Instead of using a numerical index, you can also use a string value for selection:

```
<parameter name="key">tick,tock</parameter>
<parameter name="foo" mode="python">
    {"tick" : 10,
      "tock" : 100}["${key}"]
</parameter>
<parameter name="bar" mode="python">
    {"tick" : 20,
      "tock" : 200}["${key}"]
</parameter></parameter>
```

```
"tick" : 10,
    "tock" : 100
}["${key}"]
- name: bar
mode: python
_: |
{
    "tick" : 20,
    "tock" : 200
}["${key}"]
```

Also default values are possible:

```
<parameter name="foo" mode="python">
    {"tick" : 10,
      "tock" : 100}.get("${key}",0)
</parameter>
```

4.2 Workdir change

Sometimes you want to execute a step outside of the normal *JUBE* directory structure. This can be done by using the work_dir-attribute inside the <step>-tag. If you use the work_dir *JUBE* does not create a unique directory structure. So you have to create this structure on your own if you need unique directories e.g. by using the *jube_variables*.

```
step:
  name: a_step
  work_dir: "bench_run/${jube_benchmark_padid}/${jube_wp_padid}_${jube_step_name}"
```

Using the *_padid variables will help to create a sorted directory structure.

JUBE does not create any symbolic links inside the changed work directories. If you want to access files, out of a dependend step, you can use a <fileset> and the rel_path_ref-attribute.

```
fileset:
  name: needed_files
  link:
    - {rel_path_ref: internal, _: dependent_step_name/a_file}
```

This will create a link inside your alternative working dir and the link target path will be seen relative towards the original *JUBE* directory structure. So here you can use the normal automatic created link to access all dependend files.

To access files out of an alternative working directory in a following step and if you created this working directory by using the *jube_variables*, you can use <code>jube_wp_parent_<parent_name>_id</code> to get the id of the parent step to use it within a path definition.

4.3 XML character handling

The JUBE XML based input format bases on the general XML rules. Here some hints for typical XML problems:

Linebreaks are not allowed inside a tag-option (e.g. <sub ... dest="...\n..."> is not possible). Inside a tag multiple lines are no problem (e.g. inside of <parameter>...</parameter>). Often multiple lines are also needed inside a <sub>. Linebreaks are possible for the dest="" part, by switching to the alternative <sub> syntax:

```
<sub source="...">
...
</sub>
```

Whitespaces will only be removed in the beginning and in the end of the whole string. So indentation of a multiline string can create some problems.

Some characters are not allowed inside an *XML* script or at least not inside a tag-option. Here are some of the typical replacments:

```
• <: &lt;
• >: &gt;
• &: &amp;
• ": &quot;
• ': &apos;
```

4.4 YAML character handling

The JUBE YAML based input format bases on the general YAML rules.

Instead of tags in the XML format the YAML format uses keys which values are a list of elements or other keys.

The files used for this example can be found inside examples/yaml.

The input file hello world.yaml:

```
benchmark: # having only a single benchmark, this key is optional
  name: hello_world
  outpath: bench_run
  comment: A simple hello world in yaml

#Configuration
  parameterset:
    name: hello_parameter
    parameter: {name: hello_str, _: Hello World}

#Operation
  step:
    name: say_hello
    use: hello_parameter # special key _ can be skipped
```

You can use different styles of writing key value pairs: In the example, the parameter is declared in one line using {}. Mutliple key value pairs can be stored per element. The main content attribute is marked by using _. As an alternative you can write the key value pairs amongst multiple lines using the same indent as the preceding line, like the key do in the example. If a key like use has only a value, you can write it in one line without using the special _ key.

Is list of elements can be specified by using [] or by using – amongst multiple lines (always keeping the same indent).

YAML also has a number of special characters which can be integrated by using quotation marks:

The input file special_values.yaml:

```
name: special values
outpath: bench_run
comment: An example for values that need to be in quotations
parameterset:
 name: special_parameters
 parameter:
    - {name: integer, type: int, _: "1,2,4"} #comma seperated values need to be_
→ auoted
    - {name: "NUMBER", _: "#3"} #values with # need to be quoted
patternset:
 name: special_pattern
 pattern:
    - {name: result, type: int, _: "Result: test"} #values with : need to be quoted
    - {name: integers, type: int, _: "Integers = {$integer}"} #values with {} need_
→to be quoted
    - {name: integer, type: int, _: "'Integer' = $NUMBER"} #values with ' need to_
→be quoted
```

Anytime you have a symbol like #, ', , ; or {} you have to enclose the entire value in quotation marks.

4.5 Analyse multiple output files

This FAQ entry is only relevant for *JUBE* versions prior version 2.2. Since version 2.2 *JUBE* automatically creates a combined result table.

Within an <analyser> you can analyse multiple files. Each <analyser> <analyse> combination will create independent result entries:

In this example the <patternset> a_patternset will be used for both files. This is ok if there are only patterns which match either the step_A stdout file or the step_B stdout file.

If you want to use a file dependent patternset you can move the use to a <file> attribute instead:

This avoids the generation of incorrect result entries. A from = . . . option is not available in this case. Instead you can copy the patternset first to your local file by using the init_with attribute.

Due to the independet result_entries, you will end up with the following result table if you mix the extracted pattern:

The different <analyse> were not combined. So you end up with independet result lines for each workpackage. *JUBE* does not see possible step dependencies in this point the user has to set the dependencies manually:

Now we only have one <analyse> and we are using the autogenerated link to access the dependent step. This will create the correct result:

4.6 Extract data from a specifc text block

In many cases the standard program output is structured into multiple blocks:

```
blockA:
...
time=20

blockB:
...
time=30
```

Using a simple <pattern> like time=\$jube_pat_int will match all time= lines (the default match will be the first one, and *Statistic pattern values* are available as well). However in many cases a specific value from

a sepcifc block should be extracted. This is possible by using \s within the pattern for each individual newline character within the block, or by using the dotall option:

```
<pattern name="a_pattern" dotall="true">blockB:.*?time=$jube_pat_int</pattern>
```

```
pattern:
    - {name: a_pattern, dotall: true, _: 'blockB:.*?time=$jube_pat_int'}
```

This only extracts 30 from blockB. Setting dotall="true" allows to use the . to take care of all newline characters in between (by default newline characters are not matched by .).

4.7 Restart a workpackage execution

If a problem occurs outside of the general *JUBE* handling (e.g. a crashed HPC job or a broken dependency) it might be necessary to restart a specific workpackage. *JUBE* allows this restart by removing the problematic workpackage entry and using the jube continue command afterwards:

```
jube remove bechmark_directory --id <id> --workpackage <workpackage_id>
...
jube continue bechmark_directory
```

This will rerun the specific workpackage. The *JUBE* configuration will stay unchanged. It is not possible to change the paramter> or <step> configuration later on. Shared <do> operations (shared=true) will be ignored within such a rerun scenario except if all workpackages of a specific step were removed and the full step is re-executed.

COMMAND LINE DOCUMENTATION

Here you will find a list of all available JUBE command line options. You can also use:

```
jube -h
```

to get a list of all available commands.

Because of the *shell* parsing mechanism take care if you write your optional arguments after the command name before the positional arguments. You **must** use -- to split the ending of an optional (if the optional argument takes multiple input elements) and the start of the positional argument.

When using BASH you can use the jube complete mechanism to enable a command line autocompletion.

5.1 general

General commandline options (can also be used in front of a subcommand)

```
jube [-h] [-V] [-v] [--debug] [--force] [--strict] [--devel] {...}
```

- -h, --help show general help information
- -V, --version show version information
- -v, --verbose enable verbose console output (use -vv to show stdout during execution and -vvv to show log and stdout)
- **--debug** use debugging mode (no shell script execution)
- **--force** ignore any *JUBE* version conflict
- --strict force strict JUBE version check
- --devel developer mode (show complete error messages)

5.2 run

Run a new benchmark.

```
jube run [-h] [--only-bench ONLY_BENCH [ONLY_BENCH ...]]

[--not-bench NOT_BENCH [NOT_BENCH ...]] [-t TAG [TAG ...]]

[--hide-animation] [--include-path INCLUDE_PATH [INCLUDE_PATH ...]]

[-o OUTPATH] [-a] [-r] [-e]

[-m COMMENT] [--id ID [ID ...]] FILE [FILE ...]
```

- -h, --help show command help information
- --only-bench ONLY_BENCH [ONLY_BENCH ...] only run specific benchmarks given by benchmark name

- --not-bench NOT_BENCH [NOT_BENCH ...]] do not run specific benchmarks given by benchmark name
- -t TAG [TAG ...], --tag TAG [TAG ...] use specific tags when running this file. This will be used for tagging
- --hide-animation hide the progress bar animation (if you want to use JUBE inside a scripting environment)
- --include-path INCLUDE_PATH [INCLUDE_PATH ...] add additional include paths where to search for include files
- -a, --analyse run analyse after finishing run command
- -r, --result run result after finishing run command (this will also start analyse)
- -e, --exit run will exit if there is an error
- -m COMMENT, --comment COMMENT overwrite benchmark specific comment
- -o OUTPATH, --outpath OUTPATH overwrite outpath directory
- -i ID [ID ...], --id ID [ID ...] use specific benchmark id (must be >= 0)
- **FILE** [**FILE** . . .] input *XML* file

5.3 continue

Continue an existing benchmark.

```
jube continue [-h] [-i ID [ID ...]] [--hide-animation] [-a] [-r] [-e] [DIRECTORY]
```

- -h, --help show command help information
- -i ID [ID ...], --id ID [ID ...] select benchmark id, negative ids count backwards from the end; default: last found benchmark inside the benchmark directory; special ids *all* or *last* can be used
- --hide-animation hide the progress bar animation (if you want to use JUBE inside a scripting environment)
- -a, --analyse run analyse after finishing run command
- -r, --result run result after finishing run command (this will also start analyse)
- -e, --exit run will exit if there is an error

DIRECTORY directory which contains benchmarks, default: .

5.4 analyse

Run the analyse procedure.

- -h, --help show command help information
- -i ID [ID ...], --id ID [ID ...] select benchmark id, negative ids count backwards from the end; default: last found benchmark inside the benchmark directory; special ids *all* or *last* can be used
- -u UPDATE_FILE, --update UPDATE_FILE use given input XML file to update patternsets, analyser and result before running the analyse
- --include-path INCLUDE_PATH [INCLUDE_PATH ...] add additional include paths where to search for include files (when using --update)

-t TAG [TAG ...], --tag TAG [TAG ...] use specific tags when running this file. This will be used for tagging (when using --update)

DIRECTORY directory which contains benchmarks, default: .

5.5 result

Run the result creation.

- -h, --help show command help information
- -i ID [ID ...], --id ID [ID ...] select benchmark id, negative ids count backwards from the end; default: last found benchmark inside the benchmark directory; special ids *all* or *last* can be used
- -a, --analyse run analyse before running result command
- -r, --reverse reverse benchmark output order when multiple benchmarks are given
- -n, --num show only last N benchmarks
- -u UPDATE_FILE, --update UPDATE_FILE use given input XML file to update patternsets, analyser and result before running the analyse
- -s {pretty,csv,aligned}, --style {pretty,csv,aligned} overwrites table style type
- --include-path INCLUDE_PATH [INCLUDE_PATH ...] add additional include paths where to search for include files (when using --update)
- -t TAG [TAG ...], --tag TAG [TAG ...] use specific tags when running this file. This will be used for tagging (when using --update)
- -o RESULT_NAME [RESULT_NAME ...], -only RESULT_NAME [RESULT_NAME ...] only create specific results given by name

DIRECTORY directory which contains benchmarks, default: .

5.6 comment

Add or manipulate the benchmark comment.

```
jube comment [-h] [-i ID [ID ...]] [-a] comment [DIRECTORY]
```

- -h, --help show command help information
- -i ID [ID ...], --id ID [ID ...] select benchmark id, negative ids count backwards from the end; default: last found benchmark inside the benchmark directory; special ids *all* or *last* can be used
- -a, --append append new comment instead of overwrite existing one

comment new comment

DIRECTORY directory which contains benchmarks, default: .

5.5. result 55

5.7 remove

Remove an existing benchmark

```
jube remove [-h] [-i ID [ID ...]] [-f] [DIRECTORY]
```

- -h, --help show command help information
- -i ID [ID ...], --id ID [ID ...] select benchmark id, negative ids count backwards from the end; default: last found benchmark inside the benchmark directory; special ids *all* or *last* can be used
- -w WORKPACKAGE [WORKPACKAGE ...], --workpackage WORKPACKAGE [WORKPACKAGE ...] specifc workpackage id to be removed
- -f, --force do not prompt

DIRECTORY directory which contains benchmarks, default: .

5.8 info

Get benchmark specific information

```
jube info [-h] [-i ID [ID ...]] [-s STEP [STEP ...]] [-p] [-c [SEPARATOR]] 

→ [DIRECTORY]
```

- **-h, --help** show command help information
- -i ID [ID ...], --id ID [ID ...] show benchmark specific information
- -s STEP [STEP ...], --step STEP [STEP ...] show step specific information
- -c [SEPARATOR], --csv-parametrization [SEPARATOR] display only parametrization of given step using csv format, csv separator is optional
- -p, --parametrization display only parametrization of given step

DIRECTORY show directory specific information

5.9 log

Show logs for benchmark

```
jube log [-h] [-i ID [ID ...]] [-c COMMAND [COMMAND ...]] [DIRECTORY]
```

- -h, --help show command help information
- -i ID [ID ...], --id ID [ID ...] select benchmark id, negative ids count backwards from the end; default: last found benchmark inside the benchmark directory; special ids *all* or *last* can be used
- -c COMMAND [COMMAND ...], --command COMMAND [COMMAND ...] show only logs for specified commands

DIRECTORY directory which contains benchmarks, default: .

5.10 status

Show benchmark status RUNNING or FINISHED.

```
jube status [-h] [-i ID [ID ...]] [DIRECTORY]
```

- -h, --help show command help information
- -i ID [ID ...], --id ID [ID ...] select benchmark id, negative ids count backwards from the end; default: last found benchmark inside the benchmark directory; special ids *all* or *last* can be used

DIRECTORY directory which contains benchmarks, default: .

5.11 complete

Generate shell completion. Usage: eval "\$(jube complete)"

```
jube complete [-h] [--command-name COMMAND_NAME]
```

- -h, --help show command help information
- --command-name COMMAND_NAME, -c COMMAND_NAME name of command to be complete, default: program name which was used to run the complete command

5.12 help

Command help

```
jube help [-h] [command]
```

-h, --help show command help information

command to get help about

5.13 update

Check JUBE version

```
jube update [-h]
```

-h, --help show command help information

5.10. status 57

GLOSSARY

analyse Analyse an existing benchmark. The analyser will scan through all files given inside the configuration by using the given patternsets.

If no benchmark id is given, last benchmark found in directory will be used. If benchmark directory is missing, current directory will be used.

analyser_tag The analyser describe the steps and files which should be scanned using a set of pattern.

- you can use different patternsets to analyse a set of files
- only patternsets are usable
- using patternsets <use>set1, set2</use> is the same as <use>set1</use><use>set2</
- the from-attribute is optional and can be used to specify an external set source
- any name must be unique, it is not allowed to reuse a set
- the step-attribute contains an existing stepname
- each file using each workpackage will be scanned seperatly
- the use argument inside the <file> tag is optional and can be used to specify a file specific patternset;
 - the global <use> and this local use will be combined and evaluated at the same time
 - $a \; \text{from}$ ``subargument is not possible in this local ``use
- reduce is optional (default: true)
 - true: Combine result lines if iteration-option is used
 - false: Create single line for each iteration

benchmark_tag The main benchmark definition

```
<benchmark name="..." outpath="...">
...
</benchmark>
```

- container for all benchmark information
- benchmark-name must be unique inside input file

- outpath contains the path to the root folder for benchmark runs
 - multiple benchmarks can use the same folder
 - every benchmark and every (new) run will create a new folder (named by an unique benchmark id) inside this given outpath
 - the path will be relative to input file location

column_tag A line within a ASCII result table. The <column>-tag can contain the name of a pattern or the name of a parameter.

```
<column colw="..." format="..." title="...">...</column>
```

- colw is optional: column width
- title is optional: column title
- format can contain a C like format string: e.g. format=".2f"

comment Add or manipulate the comment string.

If no benchmark id is given, last benchmark found in directory will be used. If benchmark directory is missing, current directory will be used.

comment_tag Add a benchmark specific comment. These comment will be stored inside the benchmark directory.

```
<comment>...</comment>
```

complete Generate shell completion.

continue Continue an existing benchmark. Not finished steps will be continued, if they are leaving pending mode.

If no benchmark id is given, last benchmark found in directory will be used. If benchmark directory is missing, current directory will be used.

copy_tag A copy can be used to copy a file or directory from your normal filesytem to your sandbox work directory.

- source_dir is optional, will be used as a prefix for the source filenames
- target_dir is optional, will be used as a prefix for the target filenames
- name is optional, it can be used to rename the file inside your work directory (will be ignored if you use shell extensions in your pathname)
- rel_path_ref is optional
 - external or internal can be chosen, default: external
 - external: rel.-paths based on position of xml-file
 - internal: rel.-paths based on current work directory (e.g. to link files of another step)
- active is optional
 - can be set to true or false or any Python parsable bool expression to enable or disable the single command
 - parameter are allowed inside this attribute
- each copy-tag can contain a list of filenames (or directories), separated by , , the default separator can be changed by using the separator attribute
 - if name is present, the lists must have the same length
- you can copy all files inside a directory by using $\texttt{directory}/\star$

- this cannot be mixed using name
- in the execution step the given files or directories will be copied

database_tag Create sqlite3 database

- "name": name of the table in the database
- "<key>" must contain an single parameter or pattern name
- "primekeys" is optional: can contain a list of parameter or pattern names (separated by ,). Given parameters or patterns will be used as primary keys of the database table. All primekeys have to be listed as a "<key>" as well. Modification of primary keys of an existing table is not supported. If no primekeys are set then each *jube result* will add new rows to the database. Otherwise rows with matching primekeys will be updated.
- "file" is optional. The given value should hold the full path to the database file. If the file including the path does not exists it will be created. Absolute and relative paths are supported.
- "filter" is optional. It can contain a bool expression to show only specific result entries.

directory_structure

- every (new) benchmark run will create its own directory structure
- every single workpackage will create its own directory structure
- user can add files (or links) to the workpackage dir, but the real position in filesystem will be seen as a blackbox
- general directory structure:

```
benchmark_runs (given by "outpath" in xml-file)
+- 000000 (determined through benchmark-id)
  +- 000000_compile (step: just an example, can be arbitrary chosen)
     +- work (user environment)
     +- done (workpackage finished information file)
     +- ... (more jube internal information files)
  +- 000001_execute
     +- work
        +- compile -> ../../000000_compile/work (automatic generated link,
→for depending step)
     +- wp_done_00 (single "do" finished, but not the whole workpackage)
     +- ...
  +- 000002 execute
  +- result (result data)
  +- configuration.xml (benchmark configuration information file)
  +- workpackages.xml (workpackage graph information file)
  +- analyse.xml (analyse data)
+- 000001 (determined through benchmark-id)
  +- 000000_compile (step: just an example, can be arbitrary chosen)
  +- 000001_execute
  +- 000002_postprocessing
```

do tag A do contain a executable *Shell* operation.

```
<do stdout="..." stderr="..." active="...">...</do>
<do done_file="..." error_file="...">...</do>
<do break_file="...">...</do>
<do shared="true">...</do>
<do work_dir="...">...</do>
```

- do can contain any *Shell*-syntax-snippet (*parameter* will be replaced ... \$nameofparameter ...)
- stdout- and stderr-filename are optional (default: stdout and stderr)
- work_dir is optional, it can be used to change the work directory of this single command (relativly seen towards the original work directory)
- active is optional
 - can be set to true or false or any *Python* parsable bool expression to enable or disable the single command
 - parameter are allowed inside this attribute
- done_file-filename and error_file are optional
 - by using done_file the user can mark async-steps. The operation will stop until the script will create the named file inside the work directory.
 - by using error_file the operation will produce a error if the named file can be found inside
 the work directory. This feature can be used together with the done_file to signalise broken
 async-steps.
- break_file-filename is optional
 - by using break_file the user can stop further cycle runs. the current step will be directly marked with finalized and further <do> will be ignored.
- shared="true"
 - can be used inside a step using a shared folder
 - cmd will be executed inside the shared folder
 - cmd will run once (synchronize all workpackages)
 - \$jube_wp_... parameter cannot be used inside the shared command

fileset_tag A fileset is a container to store a bundle of links and copy commands.

```
<fileset name="..." init_with="...">
  <link>...</link>
  <copy>...</copy>
  <prepare>...
...
</fileset>
```

- init_with is optional
 - if the given filepath can be found inside of the JUBE_INCLUDE_PATH and if it contains a fileset
 using the given name, all link and copy will be copied to the local set
 - the name of the external set can differ to the local one by using init-with="filename. xml:external_name"
- link and copy can be mixed within one fileset (or left)
- filesets can be used inside the step-command

general_structure_xml

```
<?xml version="1.0" encoding="UTF-8"?>
<!-- Basic top level JUBE structure -->
 <!-- optional additional include paths -->
 <include-path>
   <path>...</path>
 </include-path>
 <!-- optional benchmark selection -->
 <selection>
   <only>...</only>
   <not>...</not>
 </selection>
 <!-- global sets -->
 <parameterset name="">...</parameterset>
 <substitutionset name="">...</substitutionset>
 <fileset name="">...</fileset>
 <patternset name="">...</patternset>
 <benchmark name="" outpath="">
   <!-- optional benchmark comment -->
   <comment>...</comment>
   <!-- local benchmark parametersets -->
   <parameterset name="">...</parameterset>
   <!-- files, which should be used -->
   <fileset name="">...</fileset>
   <!-- substitution rules -->
   <substituteset name="">...</substituteset>
    <!-- pattern -->
   <patternset name="">...</patternset>
   <!-- commands -->
   <step name="">...</step>
   <!-- analyse -->
   <analyser name="">...</analyser>
   <!-- result -->
   <result>...</result>
   . . .
 </benchmark>
  . . .
</jube>
```

general_structure_yaml

```
# optional additional include paths
include-path:
...

# optional benchmark selection
selection:
only: ...
not: ...

# global sets
parameterset:
...
```

```
substitutionset:
fileset:
patternset:
benchmark: # can be skipped if only a single benchmark is handled
  - name: ...
   outpath: ...
    # optional benchmark comment
    comment: ...
    # local sets
    parameterset:
    substitutionset:
    fileset:
    patternset:
      . . .
    # commands
    step:
    analyser:
      . . .
    result:
```

include-path_tag Add some include paths where to search for include files.

```
<include-path>
  <path>...</path>
  ...
</include-path>
```

• the additional path will be scanned for include files

include_tag Include XML-data from an external file.

```
<include from="..." path="..." />
```

- <include> can be used to include an external XML-structure into the current file
- can be used at every position (inside the < jube>-tag)
- path is optional and can be used to give an alternative xml-path inside the include-file (default: root-node)

info Show info for the given benchmark directory, a given benchmark or a specific step.

If benchmark directory is missing, current directory will be used.

iofile_tag A iofile declare the name (and path) of a file used for substitution.

```
<iofile in="..." out="..." />
```

- in and out filepath are relative to the current work directory for every single step (not relative to the path of the inputfile)
- in and out can be the same

- out_mode is optional, can be w or a (default: w)
 - w: out-file will be overridden
 - a : out-file will be appended

jube_pattern List of available jube pattern:

- \$jube_pat_int: integer number
- \$jube_pat_nint: integer number, skip
- \$jube_pat_fp: floating point number
- \$ jube pat nfp: floating point number, skip
- \$jube_pat_wrd: word
- \$jube_pat_nwrd: word, skip
- \$jube_pat_bl: blank space (variable length), skip

jube_variables List of available jube variables:

· Benchmark:

- \$jube_benchmark_name: current benchmark name
- \$jube_benchmark_id: current benchmark id
- \$jube_benchmark_padid: current benchmark id with preceding zeros
- \$jube_benchmark_home: original input file location
- \$jube_benchmark_rundir: main benchmark specific execution directory
- \$ jube benchmark start: benchmark starting time

• Step:

- \$jube_step_name: current step name
- \$jube_step_iterations: number of step iterations (default: 1)
- \$jube_step_cycles: number of step cycles (default: 1)

• Workpackage:

- \$jube_wp_id: current workpackage id
- \$jube_wp_padid: current workpackage id with preceding zeros
- \$jube_wp_iteration: current iteration number (default: 0)
- \$jube_wp_parent_<parent_name>_id: workpackage id of selected parent step
- \$jube_wp_relpath: relative path to workpackage work directory (relative towards configuration file)
- \$jube_wp_abspath: absolute path to workpackage work directory
- \$jube_wp_envstr: a string containing all exported parameter in shell syntax:

```
export par=$par
export par2=$par2
```

- \$ jube wp envlist: list of all exported parameter names
- \$jube_wp_cycle: id of current step cycle (starts at 0)

key_tag A syslog result key. <key> must contain an single parameter- or patternname.

```
<key format="..." title="...">...</key>
```

• title is optional: alternative key title

• format can contain a C like format string: e.g. format=".2f"

link_tag A link can be used to create a symbolic link from your sandbox work directory to a file or directory inside your normal filesystem.

- source_dir is optional, will be used as a prefix for the source filenames
- target_dir is optional, will be used as a prefix for the target filenames
- name is optional, it can be used to rename the file inside your work directory (will be ignored if you use shell extensions in your pathname)
- rel_path_ref is optional
 - external or internal can be chosen, default: external
 - external: rel.-paths based on position of xml-file
 - internal: rel.-paths based on current work directory (e.g. to link files of another step)
- active is optional
 - can be set to true or false or any Python parsable bool expression to enable or disable the single command
 - parameter are allowed inside this attribute
- each link-tag can contain a list of filenames (or directories), separated by ,, the default separator can be changed by using the separator attribute
 - if name is present, the lists must have the same length
- in the execution step the given files or directories will be linked

log Show logs for the given benchmark directory or a given benchmark.

If no benchmark id is given, last benchmark found in directory will be used. If benchmark directory is missing, current directory will be used.

parameter_space The parameter space for a specific benchmark run is the bundle of all possible parameter combinations. E.g. there are to different parameter: a = 1,2 and b= "p","q" then you will get four different parameter combinations: a=1, b="p"; a=1, b="q"; a=2, b="p"; a=2, b="q".

The parameter space of a specific step will be one of these parameter combinations. To fulfill all combinations the step will be executed multible times (each time using a new combination). The specific combination of a step and an expanded parameter space is named *workpackage*.

parameter_tag A parameter can be used to store benchmark configuration data. A set of different parameters will create a specific parameter environment (also called *parameter space*) for the different steps of the benchmark.

```
<parameter name="..." mode="..." type="..." separator="..." export="..."

→ update_mode="..." duplicate="...">...</parameter>
```

- a parameter can be seen as variable: Name is the name to use the variable, and the text between the tags will be the real content
- name must be unique inside the given parameterset
- type is optional (only used for sorting, default: string)
- mode is optional (used for script-types, default: text)
- separator is optional, default: ,
- export is optional, if set to true the parameter will be exported to the shell environment when using <do>

- if the text contains the given (or the implicit) separator, a template will be created
- use of another parameter:
 - inside the parameter definition, a parameter can be reused: ... \$nameofparameter ...
 - the parameter will be replaced multiple times (to handle complex parameter structures; max: 5 times)
 - the substitution will be run before the execution step starts with the current *parameter space*. Only parameters reachable in this step will be usable for substitution!
- Scripting modes allowed:
 - mode="python": allow Python snippets (using eval <cmd>)
 - mode="perl": allow Perl snippets (using perl -e "print <cmd>")
 - mode="shell": allow Shell snippets
 - mode="env": include the content of an available environment variable
 - mode="tag": include the tag name if the tag was set during execution, otherwise the content is empty
- Templates can be created, using scripting e.g.: ",".join([str(2**i) for i in range(3)])
- update_mode is optional (default: never)
 - can be set to never, use, step, cycle and always
 - depending on the setting the parameter will be reevaluated:
 - * never: no reevaluation, even if the parameterset is used multiple times
 - * use: reevaluation if the parameterset is explicitly used
 - * step: reevaluation in each new step
 - * cycle: reevaluation in each cycle (number of workpackages will stay unchanged)
 - * always: reevaluation in each step and cycle
- duplicate is optional and of relevance, if there are more than one parameter definitions with the same name within one parameterset. This duplicate option has higher priority than the duplicate option of the parameterset. duplicate must contain one of the following four options:
 - none (default): The duplicate option of the parameterset is prioritized
 - replace: Parameters with the same name are overwritten
 - concat: Parameters with the same name are concatenated
 - error: Throws an error, if parameters with the same name are defined

parameterset_tag A parameterset is a container to store a bundle of parameters.

- parameterset-name must be unique (cannot be reused inside substitutionsets or filesets)
- init_with is optional
 - if the given filepath can be found inside of the JUBE_INCLUDE_PATH and if it contains a parameterset using the given name, all parameters will be copied to the local set
 - local parameters will overwrite imported parameters

- the name of the external set can differ to the local one by using init-with="filename. xml:external_name"
- parametersets can be used inside the step-command
- parametersets can be combined inside the step-tag, but they must be compatible:
 - Two parametersets are compatible if the parameter intersection (given by the parameter-name), only contains parameter based on the same definition
 - These two sets are compatible:

```
<parameterset name="set1">
    <parameter name="test">1,2,4</parameter>
    <parameter name="test2">foo</parameter>
</parameterset>
<parameterset name="set2">
    <parameter name="test">1,2,4</parameter>
    <parameter name="test">1,2,4</parameter>
    <parameter name="test3">bar</parameter>
</parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset></parameterset>
```

- These two sets are not compatible:

- duplicate is optional and of relevance, if there are more than one parameter definitions with the same name within one parameterset. This duplicate option has lower priority than the duplicate option of the parameters. duplicate must contain one of the following three options:
 - replace (default): Parameters with the same name are overwritten
 - concat: Parameters with the same name are concatenated
 - error: Throws an error, if parameters with the same name are defined

pattern_tag A pattern is used to parse your output files and create your result data.

```
<pattern name="..." default="..." unit="..." mode="..." type="..." dotall="...

→ ">...</pattern>
```

- unit is optional, will be used in the result table
- mode is optional, allowed modes:
 - pattern: a regular expression (default)
 - text: simple text and variable concatenation
 - perl: snippet evaluation (using Perl)
 - python: snippet evaluation (using *Python*)
 - shell: snippet evaluation (using *Shell*)
- type is optional, specify datatype (for sort operation)
 - default: string
 - allowed: int, float or string
- · default is optional: Specify default value if pattern cannot be found or if it cannot be evaluated

• dotall is optional (default: false): Can be set to true or false to specify if a . within the regular expression should also match newline characters, which can be very helpfull to extract a line only after a specific header was mentioned.

patternset_tag A patternset is a container to store a bundle of patterns.

```
<patternset name="..." init_with="...">
    <pattern>...</pattern>
    ...
</patternset>
```

- · patternset-name must be unique
- init with is optional
 - if the given filepath can be found inside of the JUBE_INCLUDE_PATH and if it contains a patternset using the given name, all pattern will be copied to the local set
 - local pattern will overwrite imported pattern
 - the name of the external set can differ to the local one by using init-with="filename.xml:external_name"
- patternsets can be used inside the analyser tag
- different sets, which are used inside the same analyser, must be compatible

prepare_tag The prepare can contain any *Shell* command you want. It will be executed like a normal *<do>* inside the step where the corresponding fileset is used. The only difference towards the normal do is, that it will be executed **before** the substitution will be executed.

- stdout- and stderr-filename are optional (default: stdout and stderr)
- work_dir is optional, it can be used to change the work directory of this single command (relativly seen towards the original work directory)
- active is optional
 - can be set to true or false or any Python parsable bool expression to enable or disable the single command
 - parameter are allowed inside this attribute

remove The given benchmark will be removed.

If no benchmark id is given, last benchmark found in directory will be removed.

Only the JUBE internal directory structure will be deleted. External files and directories will stay unchanged.

If no benchmark id is given, last benchmark found in directory will be used. If benchmark directory is missing, current directory will be used.

result Create a result table.

If no benchmark id is given, last benchmark found in directory will be used. If multiple benchmarks are selected (e.g. by using --id all), a combined result view of all available benchmarks in the given directory will be created. If benchmark directory is missing, current directory will be used.

result tag The result tag is used to handle different visualisation types of your analysed data.

```
<result result_dir="...">
    <use>...</use>
    ...
    ...
    <syslog>...</syslog>
```

```
<database>...</database>
...
</result>
```

- result_dir is optional. Here you can specify an different output directory. Inside of this directory a subfolder named by the current benchmark id will be created. Default: benchmark_dir/result
- only analyser are usable
- using analyser <use>set1, set2</use> is the same as <use>set1</use><use>set2</

run Start a new benchmark run by parsing the given JUBE input file.

selection_tag Select benchmarks by name.

```
<selection>
  <only>...</only>
   <not>...</not>
   ...
</selection>
```

- · select or unselect a benchmark by name
- only selected benchmarks will run (when using the run command)
- multiple <only> and <not> are allowed
- <only> and <not> can contain a name list divided by ,

statistical_values If there are multiple pattern matches within one file, multiple files or when using multiple iterations. *JUBE* will create some statistical values automatically:

- first: first match (default)
- last: last match
- min: min value
- max: max value
- avg: average value
- std: standard deviation
- sum: sum
- cnt: counter

These variabels can be accessed within the the result creation or to create derived pattern by $variable_name_<statistic_option>e.g. ${nodes_min}$

The variable name itself always matches the first match.

status Show status string (RUNNING or FINISHED) for the given benchmark.

If no benchmark id is given, last benchmark found in directory will be used. If benchmark directory is missing, current directory will be used.

step_tag A step give a list of *Shell* operations and a corresponding parameter environment.

```
<step name="..." depend="..." work_dir="..." suffix="..." shared="..." active=

..."

export="..." max_async="..." iterations="..." cycles="..." procs="..."

do_log_file="..." prepare="...">

<use from="">...</use>

...

<do></do>
```

</step>

- parametersets, filesets and substitutionsets are usable
- using sets <use>set1, set2</use> is the same as <use>set1</use><use>set2</use>
- parameter can be used inside the <use>-tag
- the from attribute is optional and can be used to specify an external set source
- any name must be unique, it is **not allowed to reuse** a set
- depend is optional and can contain a list of other step names which must be executed before the current step
- max_async is optional and can contain a number (or a parameter) which describe how many work-packages can be executed asynchronously (default: 0 means no limitation). This option is only important if a do inside the step contains a done_file attribute and should be executed in the background (or managed by a jobsystem). In this case JUBE will manage that there will not be to many instances at the same time. To update the benchmark and start further instances, if the first ones were finished, the continue command must be used.
- work_dir is optional and can be used to switch to an alternative work directory
 - the user had to handle uniqueness of this directory by his own
 - no automatic parent/children link creation
- suffix is optional and can contain a string (parameters are allowed) which will be attached to the default workpackage directory name
- active is optional
 - can be set to true or false or any Python parsable bool expression to enable or disable the single command
 - parameter are allowed inside this attribute
- shared is optional and can be used to create a shared folder which can be accessed by all workpackages based on this step
 - a link, named by the attribute content, is used to access the shared folder
 - the shared folder link will not be automatically created in an alternative working directory!
- export="true"
 - the environment of the current step will be exported to a dependent step
- iterations is optional. All workpackages within this step will be executed multiple times if the iterations value is used.
- cycles is optional. All <do> commands within the step will be executed cycles-times
- procs is optional. Amount of processes used to execute the parameter expansions of the corresponding step in parallel.
- do_log_file is optional. Name or path of a do log file trying to mimick the do steps and the environment of a workpacakge of a step to produce an executable script.
- prepare is optional and can contain a list of other step names which are prepared by this preparation step. This preparation step is only executed when at least one of the prepared steps is available. Otherwise, this preparation step is just not executed and no error is thrown in this case, which is different compared to the depend behaviour. The prepared step is implicitly dependent (depend) of this preparation step.

sub_tag A substition expression.

```
<sub source="..." dest="..." />
```

- source-string will be replaced by dest-string
- both can contain parameter: ... \$nameofparameter ...

substituteset_tag A substituteset is a container to store a bundle of *sub* commands.

```
<substituteset name="..." init_with="...">
  <iofile/>
    ...
    <sub/>
    ...
</substituteset>
```

- init_with is optional
 - if the given filepath can be found inside of the JUBE_INCLUDE_PATH and if it contains a substituteset using the given name, all iofile and sub will be copied to the local set
 - local iofile will overwrite imported ones based on out, local sub will overwrite imported ones based on source
 - the name of the external set can differ to the local one by using init-with="filename. xml:external_name"
- substitutesets can be used inside the step-command

syslog_tag A syslog result type

- Syslog deamon can be given by a host and port combination (default port: 541) or by a socket address e.g.: /dev/log (mixing of host and address is not allowed)
- format is optional: can contain a log format written in a pythonic way (default: jube[%(process)s]: %(message)s)
- sort is optional: can contain a list of parameter- or patternnames (separated by ,). Given patterntype or parametertype will be used for sorting
- <key> must contain an single parameter- or patternname
- filter is optional, it can contain a bool expression to show only specific result entries

table_tag A simple ASCII based table ouput.

- style is optional; allowed styles: csv, pretty, aligned; default: csv
- separator is optional; only used in csv-style, default: ,
- sort is optional: can contain a list of parameter- or patternnames (separated by ,). Given patterntype or parametertype will be used for sorting
- <column> must contain an single parameter- or patternname
- transpose is optional (default: false)

• filter is optional, it can contain a bool expression to show only specific result entries

tagging Tagging is a simple way to mark parts of your input file to be includable or excludable.

- Every available <tag> (not the root < jube>-tag) can contain a tag-attribute
- The tag-attribute can contain a list of names: tag="a, b, c" or "not" names: tag="a, !b, c"
- When running JUBE, multiple tags can be send to the input-file parser:

```
jube run <filename> --tag a b
```

- <taqs> which does not contain one of these names will be hidden inside the include file
- <tags> which does not contain any tag-attribute will stay inside the include file
- "not" tags are more important than normal tags: tag="a,!b,c" and running with a b will hide the <tag> because the !b is more important than the a

types *Parameter* and *Pattern* allow a type specification. This type is either used for sorting within the result table and is also used to validate the parameter content. The types are not used to convert parameter values, e.g. a floating value will stay unchanged when used in any other context even if the type int was specified.

allowed types are:

- string (this is also the default type)
- int
- float

update Check if a newer JUBE version is available.

update_mode The update mode is parameter attribute which can be used to control the reevaluation of the parameter content.

These update modes are available:

- never: no reevaluation, even if the parameterset is used multiple times
- use: reevaluation if the parameterset is explicitly used
- step: reevaluation in each new step
- cycle: reevaluation in each cycle (number of workpackages will stay unchanged)
- always: reevaluation in each step and cycle

workpackage A workpackage is the combination of a *step* (which contains all operations) and one parameter setting out of the expanded *parameter space*.

Every workpackage will run inside its own sandbox directory!

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