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Open Monte Carlo Engine User Manual

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1 Introduction

The Open Monte Carlo Engine (OMCE) is a full featured command line Monte Carlo engine that reads a model description in xml-format and runs a Monte Carlo simulation to calculate a histogram, a best estimate (mean) and the standard uncertainty. In Addition, probabilistically symmetric or shortest coverage intervals are calculated. The OMCE can be used as an alternative method to the mainstream GUM [1] to evaluate the measurement uncertainty. The OMCE implements the Monte Carlo integration method as described in the Guide to the Expression of Uncertainty Supplement 1 [2]. The OMCE is written in Python and is public domain (open source code).

1.1 Theory of operation

The OMCE reads the model description in xml-format and creates an internal list of quantities, equations and results. It then evaluates the execution order for the equation system. A production and consumer pipeline is set up with two tasks. One task calculates a block of results and analyzes it, and the other task writes the block to a binary file and frees the memory. The pipeline stops when sufficient data are produced and completely written to the binary file. The last step is to write the histogram to a text file.

1.2 Limits and restrictions

The OMCE has the following limits and restrictions:

- The number of quantities, equations and results is not limited by the software. In practice the computer hardware, the memory and the computational power will limit the size of the model that can be simulated.
- Only explicit model equations can be simulated. OMCE does not include an equation solver.

1.3 Distribution of the OMCE

The OMCE is distributed as source code accompanied by an Windows executable (exe) file for the convenience of users who do not have Stackless Python [3] or Numpy [4] installed. The OMCE was developed with Stackless Python 2.5 but should run with other Stackless Python versions as well.

1.4 Copyright

The OMCE is free software with no copyright associated with it. It can be freely copied, modified and used, but it cannot be copyrighted. The idea is to have a Monte Carlo engine that can be freely studied and modified to user needs.

1.5 Disclaimer

This software was developed at the National Institute of Standards and Technology by employees of the Federal Government in the course of their official duties. Pursuant to title 17 Section 105 of the United States Code this software is not subject to copyright protection and is in the public domain. This software is experimental. NIST assumes no responsibility whatsoever for its use by other parties, and makes no guarantees, expressed or implied, about its quality, reliability, or any other characteristic. We would appreciate acknowledgement if the software is used.

2 Installing OMCE

OMCE is distributed as a zip-file (**OMCE-1.1.14.zip**) containing all necessary files to run it on a Windows platform without Python. The zip-file should be unpacked in a separate directory **OMCE**. The OMCE can be executed directly from the command line if the **OMCE\bin** subdirectory is added to the search path. The executable version (exe) contains all packages needed to run it. In addition, the source code is included. Linux users should use the source code version. The OMCE source code makes use of Stackless Python [3] and several non-standard open source Python packages imported in the beginning of OMCE.py. The packages must be installed before the source code version can be run.

Contents of OMCE-1.1.14.zip		
File	Location	Description
OMCE.exe	OMCE\bin\	Exe version of the OMCE
OMCE.xsd	OMCE\bin\	xml schema definition of the OMCE format
OMCE.ofd	OMCE\bin\	OMCE statistical output file definition
OMCE.vfd	OMCE\bin\	OMCE var file definition
ALT.ofd	OMCE\bin\	alternative statistical output file definition
ALT.vfd	OMCE\bin\	alternative var file definition
*. *	OMCE\bin\	python runtime environment
OMCE.pdf	OMCE\doc\	OMCE user manual
OMCE\Schema.html	OMCE\doc\	OMCE xml schema description
OMCE.py	OMCE\src\	OMCE Python source file
OMCE.xsd	OMCE\src\	xml schema definition of the OMCE format
OMCE.ofd	OMCE\src\	OMCE statistical output file definition
OMCE.vfd	OMCE\src\	OMCE var file definition
ALT.ofd	OMCE\src\	alternative statistical output file definition
ALT.vfd	OMCE\src\	alternative var file definition
Viewer.py	OMCE\src\	histogram viewer
Viewer.exe	OMCE\Viewer\	EXE-version of the histogram viewer
*. *	OMCE\Viewer\	python run-time environment for the viewer
*.omc	OMCE\examples\	example xml files in OMCE format
*.xml	OMCE\examples\	example xml files in alternative format
!run_all_OMCE.bat	OMCE\examples\	batch file to run all examples in OMCE format
!run_all_ALT.bat	OMCE\examples\	batch file to run all examples in alternative format
*.ohd	OMCE\examples\ref\	reference results for the examples in OMCE format (-seed=1)
*.sta	OMCE\examples\ref\	reference results for the examples in alternative format (-seed=1)

After the installation, the windows batch file **!run_all_OMCE.bat** or **!run_all_ALT.bat** in **OMCE\examples** should be run to verify the installation. This will run the example xml files and compare the results with the reference results stored in **OMCE\examples\ref**. The random number generator is seeded for these runs so the results must exactly match the reference results.

3 Running OMCE

The OMCE is a command line tool which is designed to be used in batch scripts or to be called by other programs. If the directory of OMCE (exe-version) is included in the path, it can be executed with the following command:

```
OMCE filename.omc
```

This will start the OMCE, loading **filename.omc** and creating a file named **filename.ohd**. All options have default values. If no file name is given, a list of options with their default values and the implemented error codes is printed.

The general format for using the OMCE is:

OMCE <filename.omc>|<filename.xml> [<options>] [<parameters>]

The input file should be either in omc-format or in the alternative xml-format. See option **-fi** and Section 4.1 on file formats for more details.

All option follow the following format:

-<option>=<value>

The option name <option> is string of one to four characters identifying the option and is always followed by an equal sign. The format of the <value> depends on the option and can be either an integer, a floating point number or a string. See Section 3.1 for a detailed discussion.

Parameters have the following format:

<name>=<value>

The parameter names are defined in the omc input file (see Section 4.1.1). The value must be a floating point number.

Note: The name of the input file name must be specified before any parameters.

If there is an error, OMCE will terminate with a non-zero exit code. See Appendix A for a list of possible error messages and exit codes.

3.1 Options

The options can be given in any order but they should be separated by a space and should be given after the omc-file name.

-a This switch activates the generation of the statistical data file (.ohd) and is set to 1 by default. This switch should be set to zero if the internal data analyzer is not used and the binary data file (**-wb=1** or **-wb=2**) is analyzed by some external tool.

-ac This option controls the correlation analysis of the simulated output data.

-ac=	correlation analysis
0	no correlation analysis
1	between results (default)
2	results and their inputs
3	all

-ad This option sets the adaptive mode tolerance divisor to the value given (see section on adaptive mode). The tolerance is calculated based on the standard uncertainty or the probability interval and the number of significant digits divided by the tolerance divisor. The default value is 1.0.

The adaptive mode is controlled by the following options: **-ad**, **-af**, **-am**, **-ap**, **-at**, **-k**, **-mr**, **-sd**.

-af This option sets the probability level for the decisions during the adaptive mode. If option **-k=0** or if the alternate algorithms are used (**-am > 0**) a *t*-factor is calculated based on the probability controlled by this option and the number of simulation runs so far.

The adaptive mode is controlled by the following options: **-ad**, **-af**, **-am**, **-ap**, **-at**, **-k**, **-mr**, **-sd**.

-am This option controls the method how the number of runs are determined during the adaptive mode. The default **-am=0** uses the sequential checking scheme defined in GUM Supplement 1. Alternatively, **-am > 0** activates alternative 2-stage schemes to predict the total number of runs.

-am=	adaptive algorithm used during simulation
0	GUM Supplement 1 based algorithm
1	modified Stein 2-Stage scheme (see [5]) with S1 accuracy definition
2	modified Stein 2-Stage scheme (see [5]) with fixed relative accuracy definition
3	prediction of the needed runs with S1 accuracy definition
4	prediction of the needed runs with fixed relative accuracy definition

The adaptive mode is controlled by the following options: **-ad**, **-af**, **-am**, **-ap**, **-at**, **-k**, **-mr**, **-sd**.

- ap** This option sets the probability of the interval which is used for the tolerance check in the adaptive mode. This interval is calculated for every block of data. If bit 2 of the option **-at** is set then the standard deviation of the average of all calculated intervals is multiplied by the k -factor (option **-k**) and compared with the tolerance based on option **-sd** and **-ad**.

The adaptive mode is controlled by the following options: **-ad**, **-af**, **-am**, **-ap**, **-at**, **-k**, **-mr**, **-sd**.

- at** This option controls in detail which parameter is used to for the check in the adaptive mode (see Section 6). The value of this option is a bit combination which enables the different checks. The default is to the check the standard deviation of the mean, the standard uncertainty and the limits.

-at=	parameter used during the check
1	standard deviation of the means
2	standard deviation of the uncertainty
3	standard deviation of the means and the uncertainty (see [2] Section 7.9.4 Note 5)
7	standard deviation of the means, the uncertainty and the limits (default see [2] Section 7.9.4)

- bs** The internal data processing in the OMCE operates on data blocks with a fixed block size. The block size has influence on the performance and the statistical properties of the result. Usually the default block size (10000 values) is a good compromise between performance and statistical rigor. The block size can be changed for experimental purposes or if the value of option **-n1** or **-nc** is reduced.

In the adaptive mode the block size is adjusted automatically and the value given with this option will be overridden.

- c1** This option controls the lower limit of the absolute value of the calculated correlation coefficient. The default value is 0.001.

- da** By default (**-da=0**) an existing output file will be replaced by new simulation data. If this option is set to **-da=1**, no header is printed to the file and the data is appended. If the data should be distinguishable from prior existing data, set the option **-sid** to a different start value. Warning: The format of the existing output file will not be checked.

- de** This option controls how the name of the output files is formed from the given input filename. If this option is set (default), the extension (.omc) is deleted from the filename before the output file extension is added; otherwise the extension is added without deletion. Warning: any existing output file (.dat, .bin, .ohd, .sta) will be overwritten without warning.

- e1** The OMCE will automatically try to correct for small negative eigenvalues in the correlation matrix. This option controls the limit for the correction. The value must be negative and the default is -0.1.

- e2** When the correlation matrix needs to be corrected, the Least Maximum Norm of the correction is calculated. This option controls the limit for this norm. The default value is 0.01.

- fi** The OMCE supports two input formats which are both based on xml. The native OMCE format allows a simple description of the evaluation model. The details of the format can be found in OMCE_schema.html. As an alternative, OMCE can read an alternative xml-format.

-fi=	input format
0	OMCE format (default)
1	alternative xml-format

- fo** As a default, OMCE forms the output file name based on the given input file name. With this option an explicit output file name can be given.
- hc** The resolution of the histogram is set by this option (number of bars). The value should be between 1 and 100000. The default is 200 bars.
- hf** The width of the histogram is extended by the factor given with this option. The value should be between 0.1 and 100.0. The default is 1.2.
- hp** The width of the histogram is controlled by a probability interval to capture the relevant part of the distribution. The probability of the interval should be given as a value between 0.001 and 1. A value of 1 creates an interval that contains all values calculated during the simulation. The default is 0.99 (99 %).
- i** This options controls the interpretation of the coverage intervals. By default (-i=0), all coverage intervals are probabilistically symmetric. If the option is non-zero then the shortest coverage intervals are calculated.
- info** If the info option is non zero, OMCE prints details about the xml input file or some internal tables and quits.

-info=	description
0	(no information)
1	details of the model given in the xml-file: input quantities equations execution order results
2	list of predefined symbols and functions
3	list of symbols usable in format definition files
4	list of reserved words not to be used as quantity names
5	list of error messages in LaTeX format

- io** This option controls the sampling for imported quantities (see element `<Import>` in Section 4.1.9). If `-io=0` (default) then the binary data is sampled at random from binary files. If `-io=1` then the data is sampled sequentially from the binary file in the same (reproducible) order as it was written. If the number of runs (`-mcs`) is equal to the number of values in the binary file then the exact same sequence for the quantities is reproduced.
- k** The k-factor scales the tolerance check during the adaptive mode. The default value is 2.0. A larger value will require more Monte Carlo runs. If this option is set to zero, the k-factor will be evaluated from a *t*-table (see option `-ap`) look up based on the number of runs so far. The adaptive mode is controlled by the following options: `-ad`, `-af`, `-am`, `-ap`, `-at`, `-k`, `-mr`, `-sd`.
- l** This option allows to repeat the simulation the given number of times is it is set not equal to zero. Hint: This option is only effective if the omc-file does not contain a section `<Simulations>` and will be ignored otherwise. The default value is `-l=0`.
- lc** The correlation matrices will be printed if this option is set. The default is `-lc=0`.

-lc=	description
0	no matrix printed (default)
1	print input correlation matrix
2	print result correlation matrix
3	print input and result correlation matrix

-lmn This option defines the matrix norm type.

-lmn=	description
0	plain norm
1	weighted norm (default)

The weighted norm uses the larger correlation coefficient as a weight for the difference. The minimum weight is 0.1.

-lt If this option is set (**-lt=1**), OMCE prints the tolerances used in the adaptive mode together with the standard deviations evaluated (see section on adaptive mode for details).

-mcp This option selects the matrix correction procedure for the the correlation matrix in the event that the matrix is found to be not positive semi-definite.

-mcp=	description
0	spectral decomposition (default)
1	Near4 (N. J. Higham [6])
2	Random Walk

-mcs This option controls the number of simulation blocks. The total number of trails is the value of this option multiplied by the block size (option **-bs**). This option will override the value given in the xml-file. A value of zero or minus one activates the adaptive mode. The default value is -1.

-mr To prevent the simulation from running for an excessive amount of time during the adaptive mode, a maximum number of blocks (runs) can be set by this option. The value given here is multiplied by the block size (see option **-bs**). The default value is 10000 blocks.

The adaptive mode is controlled by the following options: **-ad**, **-af**, **-am**, **-ap**, **-at**, **-k**, **-mr**, **-sd**.

-nc This option controls the fraction of valid data that is needed to evaluate the correlation coefficients. The default value is **-nl=0.5**. The simulation is aborted if the fraction of valid data available to calculate the correlation coefficients in one data block is smaller than the value controlled by this option. Lowering this value might only be advisable if the block size is increased at the same time.

-nl This option controls the fraction of valid data that is needed to continue the simulation. The default value is **-nl=0.5**. The simulation is aborted if the fraction of valid data in one data block is smaller than the value controlled by this option. Lowering this value might only be advisable if the block size is increased at the same time.

-ofd This option controls the file name for the output format definition file. The definition file should be placed in the same directory as the OMCE executable or python source. The default is 'OMCE'.

-p1 This option controls the exact probability of the 95 % interval. The default is **-p1=0.95**.

-p2 This option controls the exact probability of the 99 % interval. The default is **-p2=0.99**.

-p3 This option controls the exact probability of the 99.9 % interval. The default is **-p3=0.999**.

-pa This option controls the exponent used for the calculation of the average of the quantiles. If a is the value set by this option then the average is calculated based on the equation

$$\bar{q} = \sqrt[a]{\frac{1}{n} \sum_{i=1}^n q_i^a}.$$

The default value is `-pa=2.0`

- pdf** The data in the histogram can either be counts (`-pdf=0`) or samples of a PDF (probability density function) (`-pdf=1`). The PDF samples are useful if the data is to be compared with a given PDF. The default is `-pdf=1`.
- po** If this option is given, OMCE will print a list of all effective options and quits. This option is useful for documenting and debugging the command line options.
- pq** This option controls the quantile estimation method. The details to the estimation methods can be found in [7].

<code>-lmn=</code>	description
0	no interpolation (see [2] Section 7.7.2) (default)
1	linear interpolation at $n_b \times p + 1/2$ (R-5)
2	linear interpolation at $(n_b + 1/3)p + 1/3$ (R-8)
3	linear interpolation at $(n_b + 1/4)p + 3/8$ (R-9)
4	linear interpolation at $(n_b + 2)p + 1/2$

- pr** The simulation is done in two steps. At the start a number of runs controlled by this option will be executed. After the first runs are completed, the binning interval and the tolerance for the adaptive mode are calculated and these values are used during the rest of the simulation runs. The default is 10 first runs.
- sbs** This option controls the sub block size for the alternate adaptive mode algorithms. The sub block mechanism is not activated by default (`-sbs=-1`). The minimum sub block size is 100. The block size must be dividable by the sub block size.
The adaptive mode is controlled by the following options: `-ad`, `-af`, `-am`, `-ap`, `-at`, `-k`, `-mr`, `-sd`.
- sd** This option controls the number of significant digits for the adaptive mode. The default is 2 digits (`-sd=2`).
The adaptive mode is controlled by the following options: `-ad`, `-af`, `-am`, `-ap`, `-at`, `-k`, `-mr`, `-sd`.
- seed** The seed of the random number generator can be set to a fixed value given by this option. A default value of zero will force a random seeding based on the system clock.
- sev** This options controls the value of the smallest eigenvalue after correction. The default is 1E-7.
- sid** This option controls the start value for the simulation ID. The default value is 0. The simulation ID will be incremented after every simulation.
- t** The OMCE will measure and print the time elapsed to run a complete simulation if `-t=1`. More detailed information on the time elapsed for the omc-file reading, simulation and the ohd-file creation will be printed if `-t=2`.
- v** This option controls the verbose level between 0 for all messages and 10 for no messages. The default value is 2.

<code>-v=</code>	description
9	error messages
8	warnings
7	startup message
6	finish message
5	simulation progress
4	timing information
3	standard information
2	default value
1	additional information and calculation details
0	everything else

Note: information requested by other options (like `-info`, etc.) will be suppressed if the verbose level is set larger as 3.

- vfd** This option gives the file name for the var-file format definition file. The definition file should be placed in the same directory as the OMCE executable or the Python source code. The default is 'OMCE'.
- vm** This option activates the validation mode if it is set. During validation mode all simulation data are kept in memory and are analysed when the simulation runs are complete.
- wb** The binary data calculated during the simulation can be written to a binary data file. This option controls the generation and the format. For the sorted format (`-wb=3`) the binary data will be sorted and made monotonic prior writing to the file. The option `-wb=3` should not be used if the data will be imported in other simulations via the element `<Import>`.

<code>-wb=</code>	format description
0	no binary data file
1	OMCE format
2	simple format
3	sorted OMCE format

The default is `-wb=0`. See the section on binary data format for details.

- wv** This option enables the creation of a .var output file. By Default no .var file is generated (`-wv=0`).
- xsd** The OMCE can validate the xml-input file against an xsd-file. With this option, the path to the xsd-file can be given. By default, the option is '-' and OMCE.xsd is used for omc-files and no validation is done for alternative xml-files. (see option `-fi`).

3.2 Example

```
OMCE S02.omc -pdf=1 -hc=400 -t=1
```

The OMCE will load the file `S02.omc` from the current directory and it will create the file `S02.ohd` containing histogram data with a resolution of 400 bins converted to a PDF sampling. The whole operation will be timed and the elapsed time will be shown.

4 OMCE file formats

The OMCE accepts two different xml-file formats discussed in the section about xml input formats. The OMCE creates data files of different types. The raw data is written to binary files and the histogram data and the other information is written to ASCII files in comma separated value format. The extension is `.ohd`.

4.1 Xml input file format

The native OMCE input file format (extension `omc`) is a simple xml-format. It describes the model of evaluation and the information about the input quantities. See `OMCE\doc\OMCE_Schema.html` for details about the omc-file format structure. An omc-file has the following basic structure:

```
<?xml version="1.0" encoding="UTF-8"?>
<Model
  Name="Model1"
  Options=""
  xmlns:xs="http://www.w3.org/2001/XMLSchema-instance"
  xs:noNamespaceSchemaLocation="OMCE.xsd">
```

```

<Parameters>
...
</Parameters>
<Quantities>
...
</Quantities>
<Correlations>
...
</Correlations>
<Functions>
...
</Functions>
<Equations>
...
</Equations>
<Constraints>
...
</Constraints>
<Results>
...
</Results>
<Simulations>
...
</Simulations>
</Model>

```

A **<Model>** element contains all information about the evaluation model. The **Name** and the **Options** attributes are optional. The **Options** attribute may contain a list of space separated command line options. The information about the schema is optional and is not used in OMCE. The validation schema is controlled by the option `-xsd`.

4.1.1 Parameters

The optional section **<Parameters>** defines a list of symbolic model parameter values that can be used in the parametric specifications of the quantities. In this section the default values of the parameters are specified. A parameter specification has the following structure:

```
<Parameter Name="P" Value="1.0"/>
```

All attributes are mandatory. The attribute **Name** defines the parameter name (e.g. "P") by which the parameter is referred to in the definition of the quantities. The attribute **Value** assigns the default value to the parameter. The value of the parameter can be re-assigned by a command line parameter (see Section 3) or inside the section **<Simulations>**.

4.1.2 Quantities

The section **<Quantities>** defines a list of quantities which can be used in the model equations. A quantity has the following structure:

```
<Quantity Symbol="X" Unit="kg"> ... </Quantity>
```

The attribute **Symbol** is mandatory and defines the symbol name (e.g. "X") by which the quantity is referred to in the equations. The attribute **Unit** is optional. A quantity element should contain one distribution element.

4.1.3 Correlations

The section `<Correlations>` is optional and defines a list of correlation coefficients which are used during the simulation runs. A correlation coefficient has the following structure:

```
<Coefficient Q1="X_1" Q2="X_2" Value="0.5" />
```

All attributes are mandatory. Attribute `Q1` and `Q2` define the quantities for the correlation coefficient and `Value` defines its value. The value must be greater than or equal to -1 and smaller than or equal to +1. All quantities where a correlation coefficient is given must be normal distributed. All correlation coefficients together must form a matrix which is positive semi-definite.

4.1.4 Functions

The section `<Functions>` is optional and defines a list of user defined functions to be used in `<Equation>` and `<Result>` elements. A function definition has the following structure:

```
<Function Symbol="f" Parameter="p1,p2" Global="X_1,X_2"> ... </Function>
```

The attribute `Symbol` is mandatory and defines the function name (e.g. "f") by which the function is referred to in `<Equation>` and `<Result>` elements. The optional attribute `Parameter` defines a parameter list for the function. The optional attribute `Global` defines a list of quantities or equation names that can be used inside the function in addition to the given parameters. The element `<Function>` should contain a valid expression.

4.1.5 Equations

The section `<Equations>` defines a list of equations which are evaluated during the simulation runs. A equation has the following structure:

```
<Equ Symbol="Y" Unit="kg"> ... </Equ>
```

The attribute `Symbol` is mandatory and defines the symbol name (e.g. "X") by which the equation is referred to in the result list or in other equations. Every equation must have a unique symbol name. The attribute `Unit` is optional. An element `<Equ>` should contain an expression which can be evaluated.

4.1.6 Constraints

The section `<Constraints>` defines a list of constraints which need to be met by the data during the simulation. A constraint has the following structure:

```
<Constraint Q="X"> ... </Constraint>
```

The attribute `Q` is mandatory and defines the name of the quantity (e.g. "X") referencing the data which is validated by the constraint. An element `<Constraint>` should contain a logical expression which can be evaluated to `True` or `False`. Logical expressions for constraints on input quantities can only refer to input quantities while logical expressions for constraints on quantities defined by equations can refer to any quantities. Quantity names referring to results cannot be used with constraints.

4.1.7 Results

The section `<Results>` defines a list of results which are observed during the simulation runs. A result has the following structure:

```
<Result Symbol="Y">Y</Result>
```

The attribute **Symbol** is mandatory and defines the symbol name (e.g. "Y") by which the result is referred to in the ohd- or var-file. The same symbol name may be used for both a result and an equation. A result element should contain a valid expression. Usually this expression contains only the name of an equation. Result symbols cannot be used in expressions for equations or results.

4.1.8 Simulations

The optional section **<Simulations>** provides a simple tool to define multiple simulations which are sequentially executed. If the section is not present in an omc-file, only one simulation is executed. All the result data for the simulations is written to the same file. The section **<Simulations>** contains a list of the elements **<Simulation>** and **<Loop>** given in any order.

The element **<Simulation>** defines one simulation run and it has the following structure:

```
<Simulation Name="Comment">
  <Parameter Name="P" Value="2.0"/>
  ...
</Simulation>
```

The attribute **Name** is optional and it specifies a comment that will be printed when the simulation is executed. The element **<Simulation>** can contain a list of parameter re-assignments. All parameter must be defined in the section **<Parameters>** before they can be used here.

The element **<Loop>** defines a for-loop for multiple simulations and it has the following structure:

```
<Loop Enum="i" From="1" To="5" Step="1.0" Name="Comment">
  <Parameter Name="P" Value="2.0*i"/>
  ...
</Loop>
```

The attribute **Enum** is optional and specifies a name for the enumerator. If the attribute is present the name given in **Enum** can be used to evaluate the values of the parameters.

The attributes **From** and **To** are mandatory and they define a range for the loop enumerator. The optional attribute **Step** specifies the value of the increment that is added (or subtracted) to the enumerator after every simulation. The default value for the **Step** is 1.0.

Note: The loop will always start with a value for the enumerator given in **From** independent if the value given in **To** is smaller or larger than **From**. The given sign of **Step** is ignored and the sign is adjusted so that the numerator is changed after every run in the direction of **To**.

The attribute **Name** is optional and specifies a comment that will be printed when the simulation is executed.

4.1.9 Distribution elements

A distribution element defines the information which is available about the quantity. The following distribution elements can be used inside a quantity element:

```
<Constant> <Value>1.0</Value> </Constant>
```

The element **<Constant>** defines a constant quantity without uncertainty.

```
<Normal> <Mean>0.0</Mean> <Sigma>1.0</Sigma> </Normal>
```

The element **<Normal>** defines a normally distributed quantity with the specified mean value and the specified standard deviation (**Sigma**).

```
<Student> <Mean>0.0</Mean> <Scalefactor>1.0</Scalefactor> <Dof>5</Dof> </Student>
```

The element **<Student>** defines a student-t distributed quantity with the specified mean value and degrees of freedom (**Dof**) scaled by the specified scaling factor (**Scalefactor**).

<Rectangle> <Mean>0.0</Mean> <Halfwidth>1.0</Halfwidth> </Rectangle>

The element <Rectangle> defines a rectangularly distributed quantity with the specified mean value and the specified half-width (semi-width).

<Triangle> <Mean>0.0</Mean> <Halfwidth>1.0</Halfwidth> </Triangle>

The element <Triangle> defines a triangularly distributed quantity with the specified mean value and the specified half-width (semi-width).

<Trapez> <Mean>0.0</Mean> <Halfwidth>1.0</Halfwidth> <Beta>0.5</Beta> </Trapez>

The element <Trapez> defines a trapezoidal distributed quantity with the specified mean value and the specified halfwidth (semi-width). Beta is the ratio between the evenly distributed part and the width of the distribution.

<Ctrapez> <Mean>0.0</Mean><Halfwidth>1.0</Halfwidth><Beta>0.5</Beta> </Ctrapez>

The element <Ctrapez> defines a iso-curvilinear trapezoidal distributed quantity [8] with the specified mean value and the specified half-width (semi-width). Beta is the ratio between the evenly distributed part and the width of the distribution.

<Ushape> <Mean>0.0</Mean> <Halfwidth>1.0</Halfwidth> </Ushape>

The element <Ushape> defines a U-shaped (arcus-sinus) distributed quantity with the specified mean value and the specified half-width (semi-width).

<TypeA> <Value>1.0</Value> ... </TypeA>

The element <TypeA> defines an observed quantity. It contains at least 2 <Value> elements.

<Poisson> <Mean>1.0</Mean> </Poisson>

The element <Poisson> defines a Poisson distributed quantity with the specified mean value.

<Exponent> <Mean>1.0</Mean> </Exponent>

The element <Exponent> defines a exponentially distributed quantity with the specified mean value.

<Gamma> <Shape>1.0</Shape> <Scale>1.0</Scale> </Gamma>

The element <Gamma> defines a Gamma distributed quantity with the specified shape and scale value.

<Discrete> <Binfile Filename="filename.bin" Index="0" Q="Y"/> </Discrete>

The element <Discrete> defines a discrete distribution based on binary data (see [2] Section 7.5.1). The element <Discrete> contains the mandatory element <Binfile> defining the binary data source. The binary data is read from a file given by the attribute **Filename**. The file should exist and it should have a valid binary format (see option **-wb**). The path should be either relative to the current XML-file or an absolute file path.

Binary files can contain binary data for multiple quantities. The optional attribute **Index** defines the index of the quantity in the binary file. The first quantity is the default and has the index 0. If the binary contains a symbol table the optional attribute **Q** can specify the name of the quantity instead of its index. The attribute **Index** will be ignored if an attribute **Q** is specified.

After the element <Binfile> two optional elements <Shift> and <Scale> can be used to define a scale value all data is multiplied with and a shift value which is added to all (shifted) values. Multiple quantities might share the same binary data with different shift and scale values. Although the these quantities share the same data, they are uncorrelated.

<Import> <Binfile Filename="filename.bin" Index="0" Q="Y"/> </Import>

The element <Import> is similar to the element <Discrete>. It contains only the element <Binfile>. No other optional elements are allowed. See the paragraph above about <Discrete> for details about the element <Binfile>. As long as only one quantity is imported per file there is virtually no difference between element <Discrete> and element <Import>. The user might use the the element <Discrete> if the distribution needs to be scaled or shifted.

If multiple quantities are imported from the same file with the element `<Import>` then the dependency structure (correlation) present in the binary data will be maintained in the current simulation by sampling jointly for all quantities from this file. Option `-io` controls if a random sampling (`-io=0`) or a sequential sampling (`-io=1`) is used.

The same binary file can be used for a `<Discrete>` element and for a `<Import>` element by using the same filenames and indices. The quantities share the distribution but they are sampled independently (not correlated).

4.1.10 Expressions and equations

The elements `<Equ>`, `<Function>` and `<Result>` require an expression as their content. The format of the expression is basically the format of a Python expression. The operator `+`, `-`, `*`, `/` and `**` can be used in expressions together with predefined functions, constants and the parentheses. The option `-info=2` lists the predefined functions and constants.

Predefined functions		
Function	Description	Remarks
<code>abs()</code>	Absolute value, Modulus	see Section 4.1.13
<code>acos()</code>	Arc cosine	
<code>asin()</code>	Arc sine	
<code>atan()</code>	Arc tangent	
<code>cos()</code>	Cosine	
<code>cosh()</code>	Hyperbolic cosine	
<code>exp()</code>	Natural exponential function (base e)	
<code>iff()</code>	Value selection	
<code>log()</code>	Natural logarithm (base e)	
<code>log10()</code>	Common logarithm (base 10)	
<code>max()</code>	Maximum value	see Section 4.1.11
<code>maximum()</code>	Maximum value	see Section 4.1.11
<code>min()</code>	Minimum value	see Section 4.1.11
<code>minimum()</code>	Minimum value	see Section 4.1.11
<code>pow()</code>	Power	see Section 4.1.12
<code>sin()</code>	Sine	
<code>sinh()</code>	Hyperbolic sine	
<code>sqr()</code>	Square	
<code>sqrt()</code>	Square root	
<code>tan()</code>	Tangent	
<code>tanh()</code>	Hyperbolic tangent	

Predefined constants		
Constant	Description	Value
<code>e</code>	Euler's number	2.7182818284590451
<code>pi</code>	number pi	3.1415926535897931

The predefined functions and constants are a direct mapping of the NumPy functions with the same name. For details consult the NumPy documentation [4]. Most of the functions except `minimum()`, `min()`, `maximum()`, `max()`, `pow()` and `iff()` have one argument. All function return one result.

OMCE allows to use distribution functions in `<Equ>`, `<Function>` and `<Result>` elements. These functions are useful to model statistical effects without assigning a quantity name to it. This is particular useful in function definitions to create certain statistically independent properties every time the function is used. All parameters of the distribution functions must evaluate to constant values by either being a numerical constant or an arithmetic expression using only quantities which are defined as constants or by using the quantity access functions `val()` or `u()` (see below).

Predefined distribution functions		
Function	Description	Parameter
Rectangle()	Rectangular distribution	Mean value, half-width
Normal()	Normal distribution	Mean value, standard uncertainty
Student()	Student-t distribution	Mean value, scale factor, degrees of freedom
Triangle()	Triangular distribution	Mean value, half-width
Trapez()	Cosine distribution	Mean value, half-width, beta factor
Ushape()	U-shaped (arcus-sinus) distribution	Mean value, half-width
Poisson()	Poisson distribution	Mean value
Ctrapez()	Iso-curvilinear trapezoidal distr.	Mean value, half-width, beta factor
Exponent()	Exponential distribution	Mean value
Gamma()	Gamma distribution	Mean value
Laplace()	Laplace distribution	Mean value, scale factor

The OMCE defines two quantity access functions to access the mean value and the standard uncertainty of named input quantities. The result of a quantity access function is a constant. These functions can be used together with the distribution functions to model dependencies between the parameters of different distributions.

Predefined quantity access functions		
Function	Description	Parameter
val()	Value function to access the mean value of an input quantity	quantity name
u()	Uncertainty function to access the standard uncertainty of an input quantity	quantity name

OMCE supports evaluation models with multiple equations. The result of one equation may be used in the calculation of another equation. But no mathematical loops are allowed. It must be possible to evaluate the equation system in a linear execution order. The model will be checked for any mathematical loop before the simulation starts.

4.1.11 Function **minimum()** and **maximum()**

The functions **minimum()** (**min()**) and **maximum()** (**max()**) have one or more parameter. The result of the function is the minimum or maximum of all the given values. These functions might produce a singular value in the PDF of the result if one of the parameter is a constant.

4.1.12 Function **pow()**

The function **pow()** can be alternatively used instead of the exponential operator ******. The function has two parameters. The first is the basis and the second is the exponent.

4.1.13 Function **iff()**

The function **iff()** allows to switch between two values based on a specified condition. The function has three parameter. The first parameter is a logical expression. If the logical expression evaluates to **True** then the second parameter will be returned as a result. If the condition evaluates to **False** then the third parameter will be returned.

This function should be used with great care since it can produce serious discontinuities in the equation system. The use of this function might violate the basis for the application of GUM Supplement 1 [2] and the use is therefore not recommended. The function is provided for experimental purposes only.

4.1.14 Logical expressions

Logical expressions are used in constraints and as the first parameter of the **iff()**-function. They must evaluate to a boolean value (**True** or **False**). Usually logical expressions used in simulations compare

data with limits or other data. The following comparison operators can be used:

Comparison operators			
Comparison	Operator	Alternative operator	Remarks
equal to	<code>==</code>	<code>.eq</code>	use with care in constraints
greater than	<code>></code>	<code>.gt</code>	
less than	<code><</code>	<code>.lt</code>	
greater than or equal to	<code>>=</code>	<code>.ge</code>	
less than or equal to	<code><=</code>	<code>.le</code>	
not equal to	<code>!=</code>	<code>.ne</code>	

The characters `<` and `>` are used as special characters with XML-files and therefore cannot be entered directly in logical expressions. Use either the escape sequences `>` and `<` or the alternative dot operators instead.

Multiple comparisons can be combined with logical operators. The following operators are supported:

Logical operators	
Operator	Description
<code>and</code>	logical and
<code>or</code>	logical or
<code>not</code>	logical complement

Some examples for valid logical expressions:

```
X .ge 0
X_1 &lt; X_2
(X .ge 1) and (X .lt 2) and not(Y .lt 0)
```

The parentheses are essential when combining comparisons.

4.1.15 Symbol names

Symbol names for quantities und equations are limited to the letters A...Z, a...z, the numbers 0...9 and the underscore character ("_"). Additionally, the @-character can be used, but it will be translated to a double underscore ("__") internally (e.g. A@A is the same as A__A). Therefore the @-character and the double underscore should not be used in the same model. The following words are reserved words and cannot be used as symbol names: and, as, assert, break, class, continue, def, del, elif, else, except, exec, finally, for, from, global, if, import, in, is, lambda, not, or, pass, print, raise, return, try, while, with, yield.

4.2 Binary data file formats

During the simulation a binary data file can be written (see option `-wb`). The OMCE supports two different binary formats.

4.2.1 OMCE binary format

The native OMCE binary format is a versatile binary format optimised for reading and writing speed. It has a block structure which corresponds to the processing block size of the data generation part of the simulation engine. The OMCE binary file has the following structure:

OMCE binary file format		
header	symbol table	binary data area
8 × 4 bytes	list of symbol names	runs × results × 8 bytes

The header is 32 bytes long and contains 6×32 -bit integer values and 8 unused bytes. The header has the following structure:

OMCE binary header						
-1330463557	m results	n runs	block size b	data offset	flags	not used
32-bit int.	32-bit int.	32-bit int.	32-bit int.	32-bit int.	32 bits	2×4 bytes

The first integer in the header is a format identifier and contains the value -1330463557. The following fields describe the data structure in the binary data area and the number of bytes used for other purposes (offset to the data). The offset to the data should be a multiple of 8 bytes.

If bit 0 in the flag word is one then a symbol table is included in the binary file. If a symbol table is present, it will directly follow the header. The symbol table contains ASCII character strings with names terminated by a zero character (00). The end of the list is an empty string or two zero characters. The symbol table is padded with additional zero characters to fill a block with a size of a multiple of 8 bytes.

The binary data contains a number of data blocks. A data block contains double precision floating point values (64-bit IEEE 754-1985) for one result only. The size is determined by the block size (see option `-bs`). If more than one result is specified the first data block of the second result will follow the first data block of the first result and so on until all first data blocks for all results are written. The same scheme will be followed up to the last block of the last result. In case that the total number of runs is not a multiple of the block size b , then the last block will be smaller than the standard block size.

Binary data structure				
data block 0, result 0	...	data block 0 result m	...	data block k result m
$b \times 8$ bytes	...	$b \times 8$ bytes	...	$b_{k+1} \times 8$ bytes

A binary file reader needs to read the header first to find out about the data structure. The total number of floating point values (64-bit) in the binary file is the product of results and runs $m \times n$ given in the header. The reader can determine the number of full data blocks k by dividing the number of runs by the block size given in the header n/b (integer division). In case the total number of values is not a multiple of the block size, then the last block is smaller and has a block size b_{k+1} which can be calculated from the number of runs modulo the block size $b_{k+1} = n \bmod b$ (modulo). After reading the header the reader should either read the symbol table if it is present or skip the number of bytes specified by the data offset in the header. The binary file contains information other than result values in this area. The value of the data offset might be zero. The unused integers in the header may be used later. The reader should not rely on them to have any specific value although they are set to zero by the OMCE so long they are not used.

A binary reader can distinguish between the OMCE binary format and the simple binary format (see next section)) by the value of the first entry in the header. The OMCE header contains a special negative number in this position while the number of runs n , the first integer in simple format, should always be positive.

4.2.2 Simple binary format

The simple binary format is an interleaving format like the OMCE format but with a fixed block size of 1 value per block. The simple binary file has the following structure:

Simple binary file format						
Header	result 0, value 0	result 1, value 0	...	result 0, value 1	...	result n, value m
2×4 bytes	8 bytes	8 bytes	...	8 bytes	...	8 bytes

The header contains 2×32 -bit integer values and is followed by a series of alternating values for all results. The header has the following structure:

Simple binary header	
n runs	m results
32-bit integer	32-bit integer

A binary file reader for the simple format may read the header first to find out about the number of runs and the number of results in the data file. While reading the data file the reader might separate the values for the different results and form larger blocks of binary values per result to optimize the later data handling. Reading and writing in simple format is less efficient than in OMCE format. The conversion from internal arrays in OMCE to the simple interleaving format of one value per block and back consumes significant computational effort.

4.3 Text data file format

OMCE supports the generation of two different output files in comma separated value format. The `ohd`-file contains the histogram data and the `var`-file contains the link between the binary data file and the result quantity names given in the model description in the `omc`-file or `xml`-file and optional correlation information. An `ohd`-file is generated when `-a=1` is activated (default) and a `var`-file is generated when `-wv` is set (deactivated by default). If a binary data file is written `-wb <> 0` then option `-wv=1` should be set as well.

The content and the format of the text files (`.var` and `.ohd`) can be customized (see option `-ofd` and `-vfd`). The format of the different text output files is controlled by format definition files. The format definition files are text files themselves and they have a line based format. Every line in a format definition file is either a comment (starting with `'#'`), an option (starting with `'-'`) or a column definition (having an equal sign). All lines which are not options and do not contain an equal sign are ignored.

This is the format definition for the OMCE `var`-file format:

```
#
# Native OMCE var-file format definition
#
-separator=", "
-header=1
-extension=".var"
-quotechar="
SID=SID
ID=id
Symbol=name
Runs=runs
Binfile=filename
R[%s]=CORR
```

It defines a comma separated text file with the file name extension `.var`. The file has a header row and 5 or more columns named `SID`, `ID`, `Symbol`, `Runs`, `Binfile` and `R[0]` to `R[n-1]` for n results.

The following options should be used in the format definition files:

- extension** This option defines the extension to the output file name. The extension should start with a point on the line. The value should be put into quotes.
- header** This option controls whether or not the file contains a header line with the column headings. A value not equal 0 will generate a header line.
- quotechar** This option controls the quoting character. No quotes should be used with this option.
- separator** This option controls the character to separate the columns in the data file. Use the combination `\t` for the tab-character. The value should be put into quotes.

All lines which are neither a comment nor contain an option define a column in the data file if they contain an equal sign. The column name will be the string left of the equal sign and the content of the column is evaluated from the string right of the equal sign. The right side should contain a predefined symbol (see option `-info=3` for a list of implemented symbols and the source code for details).

The symbol BINS, CORR and IRCORR are used to specify the histogram data and correlation data. The string left of the equal sign must contain the sequence %s which will be replaced by an ident number or a name of an input quantity.

In case the string on the right side is quoted it will be taken literally and a fixed string is written in this column.

5 Histogram viewer

The OMCE includes a simple viewer to show the result in the text file containing the histogram. The viewer can be executed with the following command:

```
Viewer <filename.ohd> [<options>]
```

The extension of the histogram data file must be given. The viewer reads the histogram data file and shows histogram plots for the results as separate plots. The plots can be saved in various graphic formats. To run the source code version of the viewer, the python module matplotlib [9] should be installed.

5.1 Options

The viewer supports the following options:

-mark The option **-mark** specifies vertical markers in the diagram to mark for example the expectation value and the coverage interval. The value of this option must be a list of marker specifications enclosed in square brackets []. A marker specification consists of a comma separated list of four values enclosed in parenthesis defining the column name, the color, the line style and the line width of the marker. The default value is:

```
-mark=[(Mean,b,dashed,1),(Low95,b,dashed,1),(High95,b,dashed,1)]
```

The column names are referring to the names given in the ohd-file.

-max This option specifies the limit for the maximum number of plots that will be generated based on the result data file (.ohd). The default is **-max=20**. If the number of results in the result data file exceeds the limit specified with this option, only the first results are plotted.

-sid This option specifies a range selection of simulation ident numbers (SID). The format of the option is **-sid=<min sid>:<max sid>** with **<min sid>** and **<max sid>** specify the lower and upper limit of simulation id's of the results which are plotted. The separator is a colon (":"). If any of the values are omitted then the minimum respectively the maximum SID in the file will be used. This option is only useful if the result data file contains data from different simulation runs.

6 Adaptive mode

The OMCE supports the automatic determination of the total number of Monte Carlo runs by the method described in the GUM Supplement 1 section 7.9 [2] (**-am=0**, default) or by alternate algorithms discuss in section 6.2. The adaptive mode is activated if the number of Monte Carlo blocks is set to zero (see option **-mcs=0**).

6.1 GUM Supplement 1 based algorithm

The GUM S1 based algorithm performs the simulation in two steps. In the beginning a number of initial runs n_{pr} , controlled by the option **-pr**, will be executed. After the initial runs the binning intervals are calculated and OMCE continues with performing additional runs.

After every additional run the tolerances T_s , T_h and T_l are calculated. Based on these tolerances OMCE decides when to terminate the simulations. The tolerances are calculated based on the number of significant digits n_{dig} controlled by the option **-sd** and the tolerance divisor d_a controlled by the option **-ad**.

For each data block i the average y_i , the standard deviation s_i , and the interval limits h_i and l_i are calculated. Based on the n_r data blocks simulated so far, the tolerances are calculated by

$$T_s = \frac{5 \times 10^{\text{mag}(\bar{s}) - n_{\text{dig}}}}{d_a}$$

$$T_h = \frac{5 \times 10^{\text{mag}(\bar{h} - \bar{y}) - n_{\text{dig}}}}{d_a}$$

$$T_l = \frac{5 \times 10^{\text{mag}(\bar{y} - \bar{l}) - n_{\text{dig}}}}{d_a}$$

with

$$\bar{s} = \sqrt{\frac{1}{n_r} \sum_{i=1}^{n_r} s_i^2}, \quad \bar{h} = \frac{1}{n_r} \sum_{i=1}^{n_r} h_i, \quad \bar{y} = \frac{1}{n_r} \sum_{i=1}^{n_r} y_i, \quad \bar{l} = \frac{1}{n_r} \sum_{i=1}^{n_r} l_i.$$

The function $\text{mag}(x)$ returns the order of magnitude of x .

During the additional simulation runs a multiple k of the standard deviation of the mean of the three parameters s_i , h_i and l_i are compared with their tolerances. The simulation terminates if all parameters are within their limits. The multiplier k is controlled by the option **-k**. With the total number of simulation runs n_r the termination criteria are

$$b_{\text{MEAN}} = \left[\frac{k \times \text{stddev}(y_1 \dots y_n)}{\sqrt{n}} \leq T_s \right]$$

$$b_{\text{UNCERTAINTY}} = \left[\frac{k \times \text{stddev}(s_1 \dots s_n)}{\sqrt{n}} \leq T_s \right]$$

$$b_{\text{LIMITS}} = \left[\frac{k \times \text{stddev}(h_1 \dots h_n)}{\sqrt{n}} \leq T_h \right] \wedge \left[\frac{k \times \text{stddev}(l_1 \dots l_n)}{\sqrt{n}} \leq T_l \right].$$

The function $\text{stddev}(x_1, \dots, x_n)$ returns the experimental standard deviation of the valid data in the series $x_1 \dots x_n$ (see Section 10.1).

Which criterion is actually in use is controlled by the option **-at**. The value of this option is a bit combination which enables the different criteria.

$$b_{\text{TERMINATION}} = (\neg \text{bit}(0) \vee b_{\text{MEAN}}) \wedge (\neg \text{bit}(1) \vee b_{\text{UNCERTAINTY}}) \wedge (\neg \text{bit}(2) \vee b_{\text{LIMITS}}).$$

The function $\text{bit}()$ returns a logical value true if the bit in option **-at** with the number given as an argument is set and the value false otherwise. By default all termination criteria are used (**-at=7**).

6.2 Alternate algorithms

The OMCE supports alternate adaptive algorithms for the determination of the total number of Monte Carlo runs. The algorithms are chosen by the option **-am**. The standard GUM S1 algorithm is the default (**-am=0**).

The numerical accuracy of all algorithms is controlled by the same options. The number of significant digits n_{dig} are controlled by the option **-sd** and the tolerance divisor d_a is controlled by the option **-ad**. The probability level p for the test is controlled by the option **-af** and the block size n_b is controlled by the option **-bs**.

The algorithms selected with options `-am=1` and `-am=2` use a modified Stein-method [5]. After the initial n_{pr} simulation blocks controlled by option `-pr`, this methods estimates the total number of runs bases on a confidence interval.

The algorithms selected with options `-am=3` and `-am=4` are based on the fact that the numerical accuracy is in principle defined relative to the variance, which allows the exact knowledge about the number of runs needed for normally distributed results.

The accuracy definition in GUM S1 is defined as half of the least significant digit and therefore the relative accuracy is dependent on the actual digits of the uncertainty (between 0.5% for the digits "99" and 5% for digits "10") the number of runs needed to meet this specification is dependent on the digits of the uncertainty.

The algorithms selected with options `-am=1` and `-am=3` use the definition of the numerical accuracy as defined in GUM S1 while the algorithm selected with option `-am=2` and `-am=4` use always the highest accuracy (assuming the digits of the uncertainty are always "99").

The algorithm selected with option `-am=3` uses a simple scheme to adapt the number of runs according to the digits of the uncertainty.

At the end all algorithms perform a statistical test to ensure that the result meets the numerical accuracy even in cases when the results are not normally distributed.

The alternate algorithms support also the option `-at` to limit the checking of the statistical parameter to the mean (bit 0) or the variance (bit 1). Bit 2 has no function with these algorithms.

6.2.1 Sub-blocking

A sub-block mechanism is used to improve the statistical properties of the statistical evaluations. The result data blocks of size n_b are divided in sub-blocks of size n_{sb} (controlled by option `-sbs`) resulting in $n_s = n_r \times n_b / n_{sb}$ sub-blocks for n_r simulated blocks. The standard deviation of the values in sub-block number i is $s_i(y_{sb})$ and the mean value of the same block is $\bar{y}_{sb}(i)$. The degrees of freedom are improved by the ratio n_b / n_{sb} . The sub-blocking is implemented efficiently without any data copying by creating a second view on the data. The sub-blocking is advantageous compare to a reduction of the block size because the performance of a Python based simulator and the accuracy of the evaluation of the coverage intervals are dependent on a large block size (≥ 10000).

6.2.2 Establishing the statistical confidence level

As proposed in [5] OMCE uses a t -factor, based on the number of sub-blocks n_s , to achieve the numerical accuracy. As long as the sub-block mean values $\bar{y}_{sb}(i)$ and the sub-block standard deviations $s_i(y_{sb})$ can be considered as random samples of a distribution with an existing variance, the variance of the overall mean and the overall variance will be improved by a factor of n_s . Therefore it is possible to use the function $N_{sb}(s, d)$ to calculate an estimate of the number of blocks needed to achieve the numerical accuracy based on the standard deviation s and the tolerance d .

$$N_{sb}(s, d) = \max \left[\text{int} \left(\frac{n_{sb}}{n_b} \times \frac{s^2 \times t_p(n_s - 1)^2}{d^2} + 0.5 \right), 1 \right]$$

The function $\max[n_1, \dots, n_l]$ returns the maximum value of the values $n_1 \dots n_l$ and the function $t_p(n_s - 1)$ returns the t -factor based on the probability p and the degrees of freedom $n_s - 1$. In case n_s is large (> 100), the t -factor could be replaced by quantile function of a normal distribution.

6.2.3 Numerical tolerance

The numerical tolerances can be either established by using the GUM S1 definition that the tolerance is half of the least significant digit of the uncertainty or the tolerance can be defined as relative to the uncertainty of the result.

The tolerance for the mean value d_m based on the GUM S1 definition is

$$d_m = 0.5 \times \frac{10^{\text{mag}(u(y))+1} \times 10^{-n_{\text{dig}}}}{d_a}$$

and the relative tolerance is dependent on the digits of the uncertainty (between 0.5% for the digits "99" and 5% for digits "10"). The function $\text{mag}(x)$ returns the order of magnitude of x . This tolerance is used by the algorithms selected with options **-am=1** and **-am=3**.

For the algorithms selected with options **-am=2** and **-am=4**, the relative tolerance is fixed (assuming the digits of the uncertainty are always "99").

$$d_m = 0.5 \times \frac{u(y) \times 10^{-n_{\text{dig}}}}{d_a}.$$

The tolerance for the variance d_v is for all algorithms

$$d_v = 2 \times u(y) \times d_m.$$

6.2.4 Predicting the number of simulation blocks

The algorithms selected with options **-am=3** and **-am=4** are based on the fact that the relative numerical accuracy of the mean value is in principle predictable if the mean value is calculated based on random samples from a distribution which has an existing variance.

Based on the number of digits n_{dig} and the tolerance divisor d_a the relative tolerance factor m can be calculated.

$$m = 10^{n_{\text{dig}}} \times d_a$$

Assuming that the number of simulations is large ($\gg 10000$) we can assume that the mean value is normally distributed and we can use the quantiles of a normal distribution to calculate a confidence interval. The variance of the mean value is proportional to $1/n$. Therefore we can predict the number of simulation runs needed to establish the relative accuracy m . This number divided by the block size n_b and rounded to the nearest integer greater than or equal to one is the number of simulation blocks n_0 to achieve the relative accuracy $1/m$.

$$n_0 = \max \left[\text{int} \left(\frac{m^2 \times \text{norm}(1 - (1 - p)/2)^2 + n_b - 1}{n_b} \right), 1 \right]$$

The function $\text{norm}(p)$ calculates the quantile of the probability p of a normal distribution and the function $\text{int}(x)$ returns the integer part of x .

The algorithm selected with option **-am=3** uses a multiple of n_0 to adapt the number of runs to the digits of the uncertainty.

The relative accuracy m is the correct numerical accuracy for the uncertainty digits "50" based on the GUM S1 definition. The correct numerical accuracy for the uncertainty digits "99" which is needed for the algorithm selected with option **-am=4**, results in a relative accuracy of $2 \times m$ and therefore in a number of simulation blocks n_1 .

$$n_1 = \max \left[\text{int} \left(\frac{4 \times m^2 \times \text{norm}(1 - (1 - p)/2)^2 + n_b - 1}{n_b} \right), 1 \right]$$

The value of n_0 is the number of simulation blocks needed to improve the variance of the mean value by m and n_1 is the number of simulation blocks needed to improve the variance of the mean value by $2 \times m$.

6.2.5 Algorithms based on the Stein-method

The algorithms selected with options `-am=1` and `-am=2` use a modified Stein-methods [5]. After the initial n_{pr} simulation blocks controlled by option `-pr`, this methods estimate the total number of runs bases on confidence intervals for the mean and the variance using the function N_{sb} defined in Section 6.2.2.

$$n_r = \max [N_{sb}(\text{stddev}(\bar{y}_{sb}(1), \dots, \bar{y}_{sb}(n_s)), d_m), N_{sb}(\text{stddev}(s_1^2(y_{sb}), \dots, s_{n_s}^2(y_{sb})), d_v)] .$$

The methods execute $n_r - n_{pr}$ additional runs and perform at the end the statistical test discussed in Section 6.2.7.

6.2.6 Algorithms based on a prediction of the needed runs

The algorithms selected with options `-am=3` and `-am=4` are based on a prediction of the runs needed (see Section 6.2.4).

If option `-am=3` or `-am=4` are selected then option `-pr` will be ignored and a number of $n_0 \times n_b$ simulations are run as initial runs.

After the initial n_0 runs the algorithm selected with option `-am=4` executes a fixed number of $n_1 - n_0$ runs as additional runs.

The algorithm selected with option `-am=3` uses the significant digits d_u of the uncertainty of the result $u(y)$ determined by the simulations so far to evaluate the need for additional runs.

$$d_u = \frac{u(y)}{10^{\text{mag}(u(y))-1}}$$

The function $\text{mag}(x)$ returns the order of magnitude of x .

The value of d_u is used to judge if additional runs are needed.

```

if  $d_u < 10 + 10/m$  or  $d_u > 50 - 10/m$ :
    DoSimulation( $n_0$ )
    if  $d_u < 10 + 10/m$  or  $d_u > 70 - 10/m$ :
        DoSimulation( $n_0$ )
        if  $d_u < 10 + 10/m$  or  $d_u > 85 - 10/m$ :
            DoSimulation( $n_0$ )

```

The function $\text{DoSimulation}(n)$ executes n simulation blocks and m is the relative tolerance factor defined in Section 6.2.4. Hint: The value of d_u is re-evaluated after the execution of $\text{DoSimulation}()$.

After the execution of the initial runs and the additional runs in total n_r simulation blocks have been executed. At the end both algorithms perform the statistical test (see next section).

6.2.7 Statistical end test

The improved adaptive algorithms selected by the option `-am > 0` test the simulation results at the end to verify that the standard deviation of the mean and the standard deviation of the variance meet the tolerance specified by n_{dig} , d_a and p . The sub-blocking mechanism (controlled by option `-sbs`) is used to improve the statistical properties of this test (see Section 6.2.1).

The test verifies that the number of runs is greater than or equal to the square of the confidence interval based on a t -factor $t_p(n_s - 1)$ and the standard deviation divided by the square of the calculated tolerance.

The test uses the function $N_{sb}(s, d)$ defined in Section 6.2.2 with the tolerances d_m and d_v discussed in Section 6.2.3.

The minimum number of runs n_{min} ensuring that the statistical properties for the mean value and the variance are met is

$$n_{min} = \max [N_{sb}(\text{stddev}(\bar{y}_{sb}(1), \dots, \bar{y}_{sb}(n_s)), d_m), N_{sb}(\text{stddev}(s_1^2(y_{sb}), \dots, s_{n_s}^2(y_{sb})), d_v)] .$$

The function `stddev(x_1, \dots, x_n)` returns the experimental standard deviation of the valid data in the series $x_1 \dots x_n$ (see Section 10.1) and the function `max[n_1, \dots, n_l]` returns the maximum value of the values $n_1 \dots n_l$.

WAn iterative test is used to verify the statistical properties since the number of sub-blocks n_s is large (> 100).

```
while  $n_r < n_{min}$ :
    DoSimulation(1)
     $n_r = n_r + 1$ 
```

Hint: The value of n_{min} is re-evaluated after every execution of `DoSimulation()`.

In case the sub-block size is large enough ($n_{sb} \geq 200$) and the distribution of the result y is not extreme and the variance of the variance exists, one can assume a close to normal distribution for the mean values $\bar{y}_{sb}(i)$ and the variances $s_i^2(y_{sb})$ of the sub-blocks (Central Limit Theorem). In this case the standard deviations of the averages will be reduced by a factor of n_s and the total number of runs can be estimated or predicted by the algorithms very precisely. Then the statistical test at the end will find only in a small number of cases that the number of runs n_r is too small ($< 5\%$, one additional block). The need for a larger number of runs during the end test might be an indication that the Central Limit Theorem is not applicable for the specific simulation problem.

7 Running multiple simulations

The OMCE is a command line program that is designed to be used in batch mode. In case it is necessary to execute a Monte Carlo simulation several times based on the same underlying model, one can either use the batch processing of the operating system and call OMCE several times or one can use the section `<Simulations>` in the omc-file to define multiple simulations. If some of the parameters need to be changed between the runs then they must be defined in the section `<Parameters>`. Using the batch processing of the operating system has the advantage that several simulations can run in parallel and that the same batch processing could be used for different models by changing only the omc-file name. Using the section `<Simulations>` has the advantage to combine everything in one input file and to generate one output file.

The following example demonstrates the use of the section `Simulations` to repeat the simulation three times and re-assigning the value of P to 1.0, 4.0 and 9.0.

```
<Simulations>
  <Simulation Name="First">
    <Parameter Name="P" Value="1.0"/>
  </Simulation>
  <Simulation Name="Second">
    <Parameter Name="P" Value="4.0"/>
  </Simulation>
  <Simulation Name="Third">
    <Parameter Name="P" Value="9.0"/>
  </Simulation>
</Simulations>
```

Alternatively, the same result can be achieved by using the element `Loop`.

```
<Simulations>
  <Loop Name="Loop" Enum="i" From="1" To="3">
    <Parameter Name="P" Value="i*2"/>
  </Loop>
</Simulations>
```

The value of a parameter can be evaluated using mathematical operators and predefined mathematical functions.

It should be noted that the parameter re-assignment in the section **simulations** override the parameter values given in the command line. So care should be taken if a omc-file with a section **simulations** is used together with batch processing.

8 Input correlation coefficients

The matrix based on the correlations coefficients given in the omc-file should be positive semi-definite. This is checked by Cholesky decomposition and eigenvalue decomposition. In cases when the matrix found to be not positive semi-definite the matrix is corrected by the chosen correction procedure (**-mcp**). The default procedure is to shift all eigenvalues which are smaller a given limit (**-sev**) to the limit and compose a new correlation matrix. A warning message together with the values of the modified correlation matrix is printed if a modification is necessary. The modification of the matrix is controlled by applying a norm [10] to the difference of the shifted and the non-shifted matrix. The norm must be smaller than a given limit (see option **-e2**) or the engine terminates with an error message.

9 Analysis of correlation

The OMCE can analyse the correlation in the results data. The analysis is controlled by the option **-ac**. The correlation is evaluated pair-wise by

$$r(q_i, q_j) = \frac{1}{(n-1) s(q_i) s(q_j)} \sum_{l=1}^n (q_{i,l} - q_i) (q_{j,l} - q_j)$$

with $q_{i,l}$ and $q_{j,l}$ being the data of the two results with the average q_i and q_j and the standard deviation $s(q_i)$ and $s(q_j)$. The correlation is evaluated for every block and the result correlation matrix is the average over all blocks. For m results $(m^2 - m)/2$ correlation coefficients are calculated. The correlation can be printed with the option **-lc=2** or the data can be written to the output files.

10 Constraints on the domain of the functions

The evaluation models given in the section **<Equations>** might be constrained in their domain. The use of the function **sqrt()** for example forms such constraint since the argument of the function cannot be negative. Any values violating any domain of the functions involved will be marked as not valid and the values will be ignore in further calculations. In addition, constraints specified in the section **<Constraints>** might restrict the domain and invalidate some values as well. As a consequence the number of valid values per block might be smaller than the number of trails. The number of runs in the statistical data file is always the number of valid values used to evaluate the result.

Since the statistical treatment is relying on a sufficiently large number of values per block, the ratio between valid values and trails is monitored. The simulation will be aborted as soon as the ratio drops below the limit defined by **-nl** (default 50 %). It is possible to reduce this limit, but it is advisable to increase the block-size (**-bs**) at the same time to guarantee that statistical treatment has still a good performance.

The correlation analysis can only be performed based on valid common data. Any invalid values in one quantity will automatically discard the values for al quantities from the data set. The ratio between the total number of values and the number of valid values is monitored. The simulation will be aborted as soon as the ratio drops below the limit defined by **-nc** (default 50 %).

The analysis of correlation can be disabled with the option **-ac=0** if the correlation information is not needed. It is also possible to reduce the limit with option **-nc** and increase the block-size sufficiently.

Non-valid data will reduce the performance of the simulation and therefore should be avoided if possible. The result will only be calculated from the valid data and all data marked as non-valid will not contribute to the result and therefore should not be calculated at all.

10.1 Mean value and uncertainty calculation

In case some of the data in a result data block i become not valid because of constraints, the effective block size of block i is reduced ($n_{\text{eff}}(i) \leq n_b$).

The total number of simulation results n in n_r simulation blocks is

$$n = \sum_{i=1}^{n_r} n_{\text{eff}}(i)$$

and the average effective blocksize \bar{n}_{eff} is

$$\bar{n}_{\text{eff}} = \frac{1}{n_r} \sum_{i=1}^{n_r} n_{\text{eff}}(i)$$

If $y[i]$ is the set of valid results for result data block i then the effective mean value $\bar{y}_{\text{eff}}(i)$ of this set is

$$\bar{y}_{\text{eff}}(i) = \frac{1}{n_{\text{eff}}(i)} \sum_{j=1}^{n_{\text{eff}}(i)} y[i]_j$$

and the effective variance $s_{\text{eff}}^2(i)$ of the data in this set is

$$s_{\text{eff}}^2(i) = \frac{1}{n_{\text{eff}}(i) - 1} \sum_{j=1}^{n_{\text{eff}}(i)} (y[i]_j - \bar{y}_{\text{eff}}(i))^2.$$

The overall mean value of the result \bar{y} is

$$\bar{y} = \frac{1}{n} \sum_{i=1}^{n_r} n_{\text{eff}}(i) \times \bar{y}_{\text{eff}}(i)$$

and the variance $u^2(y)$ is

$$u^2(y) = \frac{1}{n - 1} \sum_{i=1}^{n_r} \sum_{j=1}^{n_{\text{eff}}(i)} (y[i]_j - \bar{y})^2$$

which is equivalent of calculating

$$u^2(y) = \frac{1}{n - 1} \left[\sum_{i=1}^{n_r} (n_{\text{eff}}(i) - 1) \times s_{\text{eff}}^2(i) + \sum_{i=1}^{n_r} n_{\text{eff}}(i) \times (\bar{y}_{\text{eff}}(i) - \bar{y})^2 \right].$$

The average of the effective variance \bar{s}_{eff}^2 is

$$\bar{s}_{\text{eff}}^2 = \frac{1}{n} \sum_{i=1}^{n_r} n_{\text{eff}}(i) \times s_{\text{eff}}^2(i).$$

The variance $s^2(\bar{y}_{\text{eff}}())$ of the block mean values $\bar{y}_{\text{eff}}(i)$ for $i = 1 \dots n_r$ is

$$s^2(\bar{y}_{\text{eff}}()) = \frac{1}{\bar{n}_{\text{eff}} \times (n_r - 1)} \sum_{i=1}^{n_r} n_{\text{eff}}(i) \times (\bar{y}_{\text{eff}}(i) - \bar{y})^2$$

and the variance of the effective variances of the sets is

$$s^2(s_{\text{eff}}^2) = \frac{1}{\bar{n}_{\text{eff}} \times (n_r - 1)} \sum_{i=1}^{n_r} n_{\text{eff}}(i) \times (s_{\text{eff}}^2(i) - \bar{s}_{\text{eff}}^2)^2.$$

The nominal variance $s_{\text{nom}}^2(\bar{y}_{\text{eff}}())$ of the block mean values $\bar{y}_{\text{eff}}(i)$ for $i = 1 \dots n_r$ is

$$s_{\text{nom}}^2(\bar{y}_{\text{eff}}()) = \frac{\bar{n}_{\text{eff}}}{n_b} \times s^2(\bar{y}_{\text{eff}}())$$

The nominal variance $s_{\text{nom}}^2(y())$ is an estimate of the variance one would have got in case all blocks would have had the nominal size n_b .

11 Testing and validation

OMCE makes use of the numerical library Numpy whenever possible. So the quality of the numerical calculations are based on this library. The library is widely used and tested and is considered reliable in the context of OMCE testing and validation.

The examples given in GUM Supplement 1 are included as examples and the results can be compared with the published results.

Output (.ohd) files for all examples can be found in `OMCE\examples\ref\`. They were generated with a seeded random generator (`-seed=1`). This is used as a basic regression test during the development and it should be used to verify the installation. The windows batch file `!run_all_OMCE.bat` runs all examples and compares the result with the reference results.

12 Performance

The OMCE is optimized for an efficient calculation of models with large equation systems. During the simulation a major part of the computational power of the system will be used. The memory consumption is dependent on the model and is about 1 MB per input quantity and result.

The binary data file can be rather large without being of much use after the simulation. By default the data file will be not created. Although the binary data file is written in parallel with the calculation, the time for writing the binary data file might contribute significantly to the overall execution time if the data calculation part is significantly faster than the data writing part. At the end the OMCE has to wait until all data blocks are written to the binary file before the simulation can be completed.

12.1 Random number generation

The OMCE uses the Mersenne Twister algorithm from the NumPy package. The Mersenne Twister algorithm has a large period ($2^{19937} - 1$), creates random floats to full 53-bit precision, and has been widely tested.

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A Program exit codes

Program exit codes	
Exit Code	Error message
001	Error: Option <opt> is not valid!
002	Error: File not found (<filename>)!
003	Error: It is not a file (<string>)!
004	Error: The histogram bins must increase monotonically.!
005	Error: Option <option> should be a number (<value>)!
006	Error: Option out of range (<option>=<from>...<to>)!
007	Error: The attribute mcsimulations is not set correctly (<value>)!
008	Error: The binary data format <number> is not supported!
009	Error: Format <format> is not supported!
010	Error: Mathematical loop in process list!
011	Error: Input quantity <name> is not defined!
012	Error: Duplicated quantity name (<name>)!
013	Error: Error in expression: <expression>!
014	Error: Quantity <name> in Result <name> is unknown!
015	Error: Model Parameter <parameter> not supported!
016	Error: Correlation matrix is not positive semi-definite!
017	Error: Quantity name unknown in correlation entry (<name>)!
018	Error: Correlations are not supported for non-Gaussian Quantities (<name>)!
019	Error: Correlation coefficient out of range r(<name>,<name>)=<value>!
020	Error: Matrix modification exceeds limit (-e2=<limit>)!
021	Error: Diagonal elements of the correlation matrix must be one [r(<name>,<name>)=<value>]!
022	Error: Quantity name <name> is a reserved symbol!
023	Error: Quantity <name>, parameter <param>, syntax error in <value>!
024	Error: Parameter of function <name>() is not a constant!
025	Error: Function <name> is used without parameter!
026	Error: Quantity unknown for val(<name>)!
027	Error: The uncertainty for a t-distribution with dof<3 is not defined in u(<name>)!
028	Error: Quantity unknown for u(<name>)!
029	Error: Grammar type not supported (<type-id>)!
030	Error: Function <name>() is used recursively in its definition!
031	Error: Quantity <name> is defined as parameter and as global in function <name>()!
032	Error: Global quantity <name> in function <name>() is not defined!
033	Error: Quantity <name> in function <name>() is not defined as parameter or global!
034	Error: Unknown command line parameter name <name>!
035	Error: Quantity <name>, parameter <param>, value <value> is not an integer!
036	Error: Quantity <name>, parameter <param>, parameter unknown in <value>!
037	Error: Quantity <name>, parameter <param>, %-character is not supported (<value>)!
038	Error: Quantity <name>, parameter <param>, syntax error in <value>!
039	Error: Quantity name <name> is a predefined function!
040	Error: Quantity name <name> is a predefined symbol!
041	Error: Quantity name <name> is a reserved name!
042	Error: Quantity name <name> is the name of a user defined function!
043	Error: Parameter name <name> is a predefined function!
044	Error: Parameter name <name> is a reserved name!
045	Error: Quantity <name> in <Discrete> or <Import> element is unknown in the bin-file <filename>!
046	Error: Index unknown!
047	Error: Result name <name> is used twice in result section!

Program exit codes	
Exit Code	Error message
001	Error: Option <opt> is not valid!
002	Error: File not found (<filename>)!
003	Error: It is not a file (<string>)!
004	Error: The histogram bins must increase monotonically!
005	Error: Option <option> should be a number (<value>)!
006	Error: Option out of range (<option>=<from>...<to>)!
007	Error: The attribute mcsimulations is not set correctly (<value>)!
008	Error: The binary data format <number> is not supported!
009	Error: Format <format> is not supported!
010	Error: Mathematical loop in process list!
011	Error: Input quantity <name> is not defined!
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013	Error: Error in expression: <expression>!
014	Error: Quantity <name> in Result <name> is unknown!
015	Error: Model Parameter <parameter> not supported!
016	Error: Correlation matrix is not positive semi-definite!
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025	Error: Function <name> is used without parameter!
026	Error: Quantity unknown for val(<name>)!
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028	Error: Quantity unknown for u(<name>)!
029	Error: Grammar type not supported (<type-id>)!
030	Error: Function <name>() is used recursively in its definition!
031	Error: Quantity <name> is defined as parameter and as global in function <name>()!
032	Error: Global quantity <name> in function <name>() is not defined!
033	Error: Quantity <name> in function <name>() is not defined as parameter or global!
034	Error: Unknown command line parameter name <name>!
035	Error: Quantity <name>, parameter <param>, value <value> is not an integer!
036	Error: Quantity <name>, parameter <param>, parameter unknown in <value>!
037	Error: Quantity <name>, parameter <param>, %-character is not supported (<value>)!
038	Error: Quantity <name>, parameter <param>, syntax error in <value>!
039	Error: Quantity name <name> is a predefined function!
040	Error: Quantity name <name> is a predefined symbol!
041	Error: Quantity name <name> is a reserved name!
042	Error: Quantity name <name> is the name of a user defined function!
043	Error: Parameter name <name> is a predefined function!
044	Error: Parameter name <name> is a reserved name!
045	Error: Quantity <name> in <Discrete> or <Import> element is unknown in the bin-file <filename>!
046	Error: Index unknown!
047	Error: Result name <name> is used twice in result section!

Program exit codes	
Exit Code	Error message
048	Error: No result defined in source file!
049	Error: Unknown symbol <name> in parameter value <value>!
050	Error: Unknown symbol in parameter value <value>!
051	Error: Double assignment for r(<name>,<name>): <value> and <value>!
052	Error: A near correlation matrix could not be found in <runs> runs!
053	Error: No. of Runs in bin-file is zero!
054	Error: Bin-file format <format-id> not supported!
055	Error: Bin-file <filename> is corrupted!
056	Error: Less than <value> % of the simulated results are valid!
057	Error: The constrain for <name>: <expression> invalidates all data!
058	Error: Output File Definition not found (<filename>)!
059	Error: Constrain for <name>: <expression> cannot be evaluated!
060	Error: Unknown command line parameter argument <argument>!
061	Error: Parameter <param> in section <Simulation> is unknown!
062	Error: Loop increment (Step) must be non-zero!
063	Error: Parameter <param> in section <Loop> is unknown!
064	Error: Error in <element> name: <text>!
065	Error: quantile estimation method is unknown for -pq=<value>!
066	Error: The sub-block size -sbs=<value> must be a multiple of 10!
067	Error: The block size -bs=<value> must be a multiple of the sub-block size -sbs=<value>!
068	Error: Result data entry '<name>' unknown in ofd-file!
069	Error: Result data entry '<name>' unknown in vfd-file!
254	Error: Internal, Matrix structure does not match!
255	Error: <error message>!