Neper Reference Manual

The documentation for Neper 4.0.2
A software package for polycrystal generation and meshing

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User Guidelines

If you use Neper for your own work, please, mention it explicitly in your reports (papers, books, talks, ...) and cite one or several of the following papers (depending of your use of Neper):

- *R. Quey, P.R. Dawson, F. Barbe. Large-scale 3D random polycrystals for the finite element method: Generation, meshing and remeshing. Comput. Methods Appl. Mech. Engrg., vol. 200, pp. 1729–1745, 2011* (for Voronoi tessellation, regularization, meshing);
- *R. Quey and L. Renversade, Optimal polyhedral description of 3D polycrystals: Method and application to statistical and synchrotron X-ray diffraction data, Comput. Methods Appl. Mech. Engrg., vol. 330, pp. 308-333, 2018* (for tessellation from custom or experimental properties with option `-morpho`);
- *R. Quey, A. Villani and C. Maurice, Nearly uniform sampling of crystal orientations, J. Appl. Crystallogr., vol. 51, pp. 1162-1173, 2018* (for uniform crystal orientation distribution with option `-ori uniform`).

1 Introduction

1.1 The Neper Project

1.1.1 Description

Neper is a software package for polycrystal generation and meshing. The polycrystals can be 2D or 3D. Neper is built around four modules:

- Module -T generates polycrystals as tessellations. The two main capabilities are: *(i)* the generation of tessellations from cell properties (e.g. a size distribution) and *(ii)* the generation of multiscale tessellations (i.e. including cell subdivisions). These capabilities can also be used together. Tessellations are Laguerre (or Voronoi) tessellations and are therefore composed of convex cells. Once generated, the tessellations can be "regularized" by removing their smallest features (edges and faces), which then enables good-quality meshing with module -M. Periodicity conditions can be prescribed. Crystal orientations are provided for the cells. The output is a tessellation file written at a scalar (vectorial) or raster format. Scalar tessellations are intended to be passed to modules -M and -V while raster tessellations can be used by FFT solvers.
- Module -M meshes polycrystals described as tessellation files. Two meshing techniques are available: free (or unstructured) meshing, which generates triangular elements (in 2D) or tetrahedral elements (in 3D) that follow the grain shapes, and mapped meshing, which generates regular, square elements (in 2D) or regular, cubic elements (in 3D) that do not necessarily follow the grain shapes. Free meshing into good-quality elements is ensured by optimized meshing rules, and multimeshing—a complementary use of several meshing algorithms. Remeshing is also available and is similar to meshing except that it takes a mesh as input. Cohesive elements can be inserted at interfaces. The output is a mesh file written in the .msh format, which can be readily used by Neper's companion program, the FEPX finite-element crystal-plasticity software package, or other formats.
- Module -S works in conjunction with FEPX to generate a simulation directory. It reformats the FEPX raw simulation results and includes various post-processing capabilities to compute new results. The resulting simulation directory can be loaded as input in module -V.
- Module -V generates publication-quality PNG images or VTK files (for interactive visualization) of tessellations, meshes and simulation results. The results can be defined from internal data, data loaded from external files, or a simulation directory as generated by module -S. For PNG images, the coloring and transparency of the different entities can be set up in great detail, and slice views can be plotted.

Neper strives to be an easy-to-use, efficient and robust tool. All the input data are prescribed non-interactively, using command lines and / or ASCII files, so that all treatments can be automated.

1.1.2 Resources and Support

Several, complementary resources describing Neper are available:

- The Neper reference manual, which is this document, describes all Neper's capabilities. Each module is dedicated a specific chapter, which describes the available commands and result files, and provides examples. The manual is available at the PDF and info formats.[1]
- The Neper website, `http://neper.info`, gives a general introduction to Neper (including examples with illustrations) and is where Neper can be downloaded from. Official versions are released on the website every few months, as zipped tarballs (`tgz` files), while the latest,

[1] Provided that the info file is properly installed at your site, it can be accessed by the command: `info neper`.

development version is available from the development repository, `https://github.com/rquey/neper`. The best way to get and keep up-to-date with development versions is to clone the repository, using

```
$ git clone https://github.com/rquey/neper.git
```

which gives access to the latest development version on the default, `devel` branch (so as to all previous development versions), but also to all official versions (which can be listed using `git tag`). To update your local repository, run `git pull` from within the repository.

- The three Neper reference papers,
  - "*R. Quey, P.R. Dawson and F. Barbe, Large-scale 3D random polycrystals for the finite element method: Generation, meshing and remeshing, Comput. Methods Appl. Mech. Engrg., vol. 200, pp. 1729-1745, 2011*" describes the regularization / meshing methodologies. It can be downloaded from the Neper homepage or directly from this link: `http://neper.info/docs/neper-reference-paper.pdf`;
  - "*R. Quey and L. Renversade, Optimal polyhedral description of 3D polycrystals: Method and application to statistical and synchrotron X-ray diffraction data, Comput. Methods Appl. Mech. Engrg., vol. 330, pp. 308-333, 2018*" describes tessellation generation from experimental properties;
  - "*R. Quey, A. Villani and C. Maurice, Nearly uniform sampling of crystal orientations, J. Appl. Crystallogr., vol. 51, pp. 1162-1173, 2018.*" describes uniform sampling of crystal orientations.

The best way to report bugs is directly through the GitHub issue tracker, `http://github.com/rquey/neper/issues`. When reporting bugs, please help us helping you by providing a minimal working example and the terminal output. Neper also has two dedicated mailing lists (the GitHub issue tracker should be preferred, especially for bug reports): `neper-announce` (`https://lists.sourceforge.net/lists/listinfo/neper-announce`), the "read-only" list for release announcement, and `neper-users` (`https://lists.sourceforge.net/lists/listinfo/neper-users`), the "read-write" list for users. As of October 2019, Neper also has an IRC channel, `#neper`, on the `freenode` network.

Resources for FEPX can be accessed from `http://fepx.info`.

1.2 Installing Neper

Neper is written in (mostly ANSI) C and a little C++, and it can run on any Unix-like system (including MacOS). Multithreading of the code is achieved via OpenMP and operates on all threads (the actual number of threads can be set throught the *`OMP_NUM_THREADS`* environment variable). Compilation is performed via CMake:

- Create a `build` directory, for instance as a subdirectory of Neper's `src` directory

  ```
  $ mkdir build
  ```

- Run CMake from within the `build` directory, pointing to Neper's `src` directory

  ```
  $ cd build
  $ cmake ..
  ```

- Build Neper

  ```
  $ make
  ```

  Use option `-j` for a multithreaded compilation.

- Install Neper on your system (as root)

  ```
  $ make install
  ```

This procedure uses the default configuration options and should work out-of-the-box if the required dependencies are available in standard system locations. If needed, a finer configuration

of which dependencies are included can be achieved, before building Neper, by setting variables `HAVE_`*`DEPENDENCY`*, where *`DEPENDENCY`* is the name of the dependency. This can be done using

```
$ ccmake ..      (for an interactive command-line tool)
```

or

```
$ cmake-gui ..  (for an interactive graphical tool)
```

or directly at the command line, by using `cmake`'s `-D` option,

```
$ cmake -DHAVE_DEPENDENCY1={ON,OFF} -DHAVE_DEPENDENCY2={ON,OFF} ..
```

The dependencies which are (optionnally) necessary at compilation time are the following:

- The GNU Scientific Library (GSL, mandatory, variable '`HAVE_GSL`'). It is likely to be available on your system or from your system package manager (binary and development packages); alternatively, the source code version can be downloaded from `http://www.gnu.org/software/gsl`.
- The NLopt library (version `2.6.0` or higher, optional, enabled by default, variable '`HAVE_NLOPT`'). It is needed by module -T for tessellation generation from cell properties. It is likely to be available on your system or from your system package manager (binary and development packages); alternatively, the source code version can be downloaded from `http://ab-initio.mit.edu/wiki/index.php/NLopt`.
- The OpenMP library (optional, enabled by default, variable '`HAVE_OPENMP`'). It is likely to be available on your system or from your system package manager.[2]
- The libScotch library (version `6.0.0` or higher, optional, disabled by default, variable *`HAVE_LIBSCOTCH`*). It is needed by module -M for mesh partitioning. The source code can be downloaded from `www.labri.fr/perso/pelegrin/scotch`.
- The pthread library (mandatory if libScotch enabled). It is likely to be available on your system or from your system package manager.

Other dependencies are only needed at run-time (they are not necessary for compilation):

- The Gmsh program (version `2.4.2` or higher, excluding version `2.5.1`, mandatory for module -M). Both binary and source-code versions can be downloaded from `http://www.geuz.org/gmsh` (compiling from the source code significantly speeds up meshing). Gmsh must be available at the terminal as the command `gmsh`, or the path to its binary must be specified with option `-gmsh` (in module -M).
- The POV-Ray program (version `3.7` or higher, mandatory for module -V). It is likely to be available on your system or from your system package manager (binary package); alternatively, a binary, or the source code, can be downloaded from `http://www.povray.org`. POV-Ray must be available at the terminal as the command `povray`, or the path to its binary must be specified with option `-povray` (in module -V).

Neper has a few more dependencies, which are directly included in the source code (see directory `src/contrib`): nanoflann (`https://github.com/jlblancoc/nanoflann`), muparser (`http://beltoforion.de/article.php?a=muparser`), openGJK (`https://github.com/MattiaMontanari/openGJK`) and tinycolormap (`https://github.com/yuki-koyama/tinycolormap`).

Finally, the Neper installation can be tested out by running

```
$ make test
```

or (equivalently)

```
$ ctest
```

[2] On Mac, install `llvm` and `libomp` via Homebrew.

1.3 Getting Started

The '`neper`' binary must be run in a terminal, followed by a list of arguments,

```
$ neper list_of_arguments
```

Neper returns messages in the terminal and results in ASCII (optionally binary) files.

The list of arguments describes the problem to solve. There are several general-purpose, self-explanatory arguments:

```
$ neper --help
$ neper --version
$ neper --license
```

The following of this section provides information on how to call Neper's modules, properly format option arguments and set up an initialization file.

1.3.1 Modules

To call a module, run

```
$ neper module_name module_arguments
```

where the module name can be `-T`, `-M`, `-S` or `-V`, and the module arguments can include both required input data and options. Input data (when not a file name) and options start by '`-`'. Options can be provided in arbitrary order, each of them being followed by a single argument (containing no space). String completion is available for all options, so they may be abbreviated as long as the abbreviation is not ambiguous. For instance, in module `-T`, option `-regularization` can be abbreviated to `-reg`. In the rare cases where an argument contains shell metacharacters (most commonly '`(`', '`)`', '`?`', etc.), it must be enclosed in either single or double quotes to be read in properly (note that only double quotes enable variable substitution by the shell). Logical options can be enabled or disabled by providing argument values of '`1`' or '`0`', respectively. Integer or real arguments can be written as numeral values, or mathematical or logical expressions (see Section A.1 [Mathematical and Logical Expressions], page 65). For instance, in module -T, option '`-rcl 0.5`' can also be written as '`-rcl 1/2`' or '`-rcl "cos(pi/3)"`'. For some options, different values can be specified to different entities by loading them from an external file, using an argument of the form '`"file(file_name)"`'. The file must contain the expected number of values and can be arbitrarily formatted in terms of delimiters (spaces, tabs or newlines). For the more complex case of a multiscale tessellation, a *multiscale cell file* can also be used, for which details are provided in Section B.3 [Multiscale Cell File], page 88. Module -V shows some exceptions with respect to these rules: the argument cannot be listed in arbitrary order, string completion is not available, and option `-loop` takes several arguments.

1.3.2 Argument Separators

Some options may take several argument values. These values can be combined using *separators* (see Chapter 2 [Tessellation Module (-T)], page 11, Chapter 3 [Meshing Module (-M)], page 29, Chapter 4 [Simulation Module (-S)], page 43, and Chapter 5 [Visualization Module (-V)], page 45, for details on each option). There are three possible separators:

- The '`,`' separator combines uncorrelated arguments, i.e. arguments of the same type, which can be processed independently from each other, in any order. This is for example the case of output file formats.
- The '`:`' separator is used to combine correlated arguments, i.e. arguments of different types, which cannot be processed independently from each other and must be processed in order. This is for example the case of the values of a variable in different directions.
- The '`::`' separator is used in module -T (and a little in module -M) for assigning argument values to the different scales of a multiscale tessellation. It is a "super-separator" that takes precedence over the '`,`' and '`:`' standard separators.

1.3.3 Initialization File

When Neper is run, it starts by reading commands from an initialization file, `$HOME/.neperrc`, if that file exists. Another initialization file can be specified with option `--rcfile`, before calling a module,

```
$ neper --rcfile my_file module_name module_arguments
```

The reading of an initialization file can be disabled use option '`--rcfile none`'.

When a Neper module is called, Neper looks for the occurrence of '`neper module_name`' in the initialization file and then reads all arguments until the next occurrence of '`neper`' (which should denote the beginning of another module option field) or the end of the file. The arguments may be any legal arguments but are typically limited to frequently-used options. Moreover, any field of comments can be preceded by '`neper comments`'.

Here is the example of an initialization file, featuring its syntax (parts beginning with '`<-- `' do not belong to the file):

```
neper comments ------------------------------------  <-- comment
This is my initialization file.                      <-- comment
                                                     <-- comment
        It's pretty incomplete though...             <-- comment
                                                     <-- comment
neper -T -reg 1                                      <-- neper -T option
neper -M -gmsh my_gmsh_path                          <-- neper -M option
     -order 2                                        <-- neper -M option
                                                     <-- comment
neper comments                                       <-- comment
        Remember to add what I don't remember!       <-- comment
neper -V -povray my_povray_path                      <-- neper -V option
neper comments ------------------------------------  <-- comment
```

If the initialization file is not found, or if '`neper module_name`' is not found inside it, Neper will consider only the command line arguments. Also, if an argument is initialized several times (for instance, both in the initialization file and at the command line), only the last specified value is used.

1.4 Reading this Manual

This manual is maintained as a Texinfo manual. Here are the writing conventions used in the document:

- A command that can be typed in a terminal is printed like `this`, or, in the case of a major command, like

  ```
  $ this ;
  ```

- A program (or command) option is printed like `this`;
- The name of a variable is printed like `this`;
- A meta-syntactic variable (i.e. something that stands for another piece of text) is printed like *this*;
- Literal examples are printed like '`this`';
- File names are printed like `this`.

Module arguments are tagged by type and importance level:

- Prerequisites are tagged '[Prerequisite]'—they should be placed in the initialization file;

- Input data are tagged '[Input Data]';
- Standard options are tagged '[Option]';
- Secondary options, which should be used only for fine-tuning and if you really know what you are doing, are tagged '[Secondary option]';
- Post-processing options are tagged '[Post-processing]'.

Some options take optional or repeated arguments, conventionally specified by using square brackets and ellipses: an argument enclosed within square brackets is optional, and an argument followed by an ellipsis is optional and may be repeated more than once.

Some abbreviations are used consistently for options and contribute to Neper's jargon:

`algo`	algorithm
`arch`	architecture
`aspratio`	aspect ratio
`cl`	characteristic length
`col`	color or column
`conv`	convergence
`coo`	coordinate
`crysym`	crystal symmetry
`csys`	coordinate system
`diameq`	equivalent diameter
`dim`	dimension
`dis`	distribution or distortion
`dof`	degree of freedom
`dup`	duplicate(d)
`elset`	element set
`elt`	element
`expr`	expression
`fact`	factor
`faset`	element face set
`geo`	geometry
`id`	identifier
`ini`	initial
`inf`	infinity
`inter`	interpolation
`iter`	iteration
`max`	maximum
`min`	minimum
`morpho`	morphology
`neigh`	neighbor
`nset`	node set
`opti`	optimization
`ori`	orientation
`part`	partition
`poly`	polyhedron
`pov`	POV-Ray file
`qual`	quality
`rad`	radius
`rcl`	relative characteristic length
`res`	resolution
`rmax`	relative maximum
`sing`	singular

`stat`	statistics
`surf`	surface
`tesr`	raster tessellation
`tess`	scalar tessellation
`tmp`	temporary
`trs`	transparency
`val`	value
`var`	variable
`ver`	vertex

2 Tessellation Module (-T)

Module -T is the module for generating *tessellations* and *multiscale tessellations* of a bounded *domain* of space, in 2D or 3D. The domain must be convex, but once generated the tessellation can be cut by various shapes, e.g. to include a notch (experimental[1]). Periodicity and semi-periodicity conditions can be prescribed. Module -T also enables the *regularization* of the tessellations for meshing with high quality elements. The tessellations are provided in scalar (vectorial) or raster formats. Module -T also generates crystal orientations for the tessellation cells.

Tessellations can be generated from various types of morphological cell properties (option `-morpho`). Several predefined properties are available, such as those obtained by grain growth in metals (which are described by cell size and sphericity (circularity, in 2D) distributions). Custom properties can be specified using various metrics, including the size and sphericity (circularity, in 2D), the centroid or even the actual shape (using a raster tessellation), in terms of either distributions (when applicable) or individual cell values. Global morphological properties, such as a cell aspect ratio or a columnar axis, can also be specified. The generated *tessellations* are Laguerre (or Voronoi) tessellations whose seed attributes are set by optimization to obtain the desired cell properties. Of course, it is also possible to generate standard tessellations (e.g. Poisson-Voronoi or regular tessellations). Cell *groups* can be defined to represent the different phases of a multiphased polycrystalline material (option `-group`).

Multiscale tessellations are characterized by the subdivision of the cells of a primary tessellation into secondary tessellations (and so on) and are obtained by combining into one, using '`::`', the option arguments that apply at the successive scales. The same value can be used for defining the tessellations at a given scale, or different values can be loaded using '`msfile(`*`filename`*`)`', where *`filename`* is a *multiscale cell file* (see Section B.3 [Multiscale Cell File], page 88).[2] So, all capabilities available for generating a standard (single-scale) tessellations are available for generating the tessellations at the different scales of a multiscale tessellation. Examples are provided in the following.

The *domain* of space in which the tessellation is created can be of any convex shape. In 3D, cuboidal, cylindrical and spherical shapes (and a few other, exotic shapes) are directly supported while other morphologies can be defined from a set of planes (option `-domain`). Non convex domain shapes can be obtained by cutting the tessellation by different geometrical primitives once generated (option '`-transform cut`', experimental).[3] Periodicity or semi-periodicity conditions can be applied to the tessellation (option `-periodicity`).

Crystal orientations can be randomly distributed (according to a uniform distribution function), either in the 3D space or along a specific orientation fibre, or uniformly distributed (also according to a uniform distribution function, option `-ori`). Uniform crystal orientation distributions ensure that all possible crystal orientations are equally represented (no orientation clustering). Crystal orientations can be written according to different descriptors (option `-oridescriptor`). It is also possible to define an analytical orientation distribution for the cells (option `-oridistrib`).

Regularization can be applied to the tessellations and consists of removing their small edges and faces (option `-regularization`) which would otherwise be detrimental to generating meshes with high quality elements with module -M (see Chapter 3 [Meshing Module (-M)], page 29).[4]

Output files describe the tessellation either at the scalar format `.tess` or at the raster format `.tesr` (see Section B.1 [Tessellation File (`.tess`)], page 81, and Section B.2 [Raster Tessellation

[1] This capability may fail as the local shape curvature approaches the cell size.

[2] As of version 3.5.0, '`msfile(`*`filename`*`)`' should be preferred to '`file(`*`filename`*`)`' to load a multiscale cell file.

[3] Only non-convexities larger than the typical cell size are supported.

[4] Not available for periodic tessellations.

File (`.tesr`)], page 86, respectively). Both are input files of module -M (see Chapter 3 [Meshing Module (-M)], page 29) and module -V (see Chapter 5 [Visualization Module (-V)], page 45). Third-party software file formats are also available.

Here is what a typical run of module -T looks like:

```
$ neper -T -n 10 -reg 1

========================    N   e   p   e   r    ======================
Info   : A software package for polycrystal generation and meshing.
Info   : Version 4.0.0
Info   : Built with: gsl|muparser|opengjk|openmp|nlopt|libscotch (full)
Info   : Running on 8 threads.
Info   : <http://neper.info>
Info   : Copyright (C) 2003-2020, and GNU GPL'd, by Romain Quey.
Info   : No initialization file found ('/home/rquey/.neperrc').
Info   : ---------------------------------------------------------------
Info   : MODULE  -T loaded with arguments:
Info   : [ini file] (none)
Info   : [com line] -n 10 -reg 1
Info   : ---------------------------------------------------------------
Info   : Reading input data...
Info   : Creating domain...
Info   : Creating tessellation...
Info   :   - Setting seeds...
Info   :   - Generating crystal orientations...
Info   :   - Running tessellation...
Info   : Regularizing tessellation...
Info   :   - loop 2/2: 100% del=14
Info   : Writing results...
Info   :     [o] Writing file 'n10-id1.tess'...
Info   :     [o] Wrote file 'n10-id1.tess'.
Info   : Elapsed time: 0.036 secs.
===============================================================================
```

2.1 Arguments

2.1.1 Input Data

`-n` *integer or char_string* [Input data]

Specify the number of cells of the tessellation. The argument can be an integer, an expression based on the tessellation cell variables (see Section A.2 [Tessellation Keys], page 67), or '`from_morpho`' to set the value from the morphology (option `-morpho`).
Possible values: `any`. Default value: `none`.

`-id` *integer* [Input data]

Specify the identifier of the tessellation. It defines the seed used by the random number generator to compute the (initial) seed positions.
Possible values: `any`. Default value: `1`.

`-dim` *integer* [Option]

Specify the dimension of the tessellation.
Possible values: `2 or 3`. Default value: `3`.

`-domain` *char_string* [Option]

Specify the domain morphology. In 3D, for a cuboidal shape, provide '`cube(size_x,size_y,size_z)`', for a cylindrical shape, provide '`cylinder(height,diameter)`', and for a spherical shape, provide '`sphere(diameter)`'. In 2D, for a rectangular shape, provide '`square(size_x,size_y)`', and for a circular shape, provide '`circle(diameter)`'. The curved shapes of circular, cylindrical and spherical domains are built on discrete linear segments and planar facets, whose number, *facet_nb*, can be specified using '`circle(diameter,facet_nb)`', '`cylinder(height,diameter,facet_nb)`' or '`sphere(diameter,facet_nb)`'. For a Rodrigues space fundamental region, provide '`rodrigues(crysym)`', where *crysym* is the crystal symmetry (see Section A.10 [Crystal Symmetries], page 76). For a standard stereographic triangle, provide '`stdtriangle(segment_nb)`', where *segment_nb* is the number of segments on the [011]–[111] line. For an arbitrary convex 3D shape, provide '`planes(file_name)`', where *file_name* is the name of a file containing the total number of planes then, for each plane, the 4 parameters of its equation: d, a, b and c, successively, for an equation of the form $a\,x + b\,y + c\,z = d$, and where the plane normal, (a, b, c), is an outgoing vector of the domain. For a tessellation cell, provide '`cell(file_name,cell_id)`', where *file_name* is the name of the tessellation file and *cell_id* is the cell identifier. To transform the domain, append a transformation to the domain name using '`:`'. Available transformations are: '`rotate(axis_x,axis_y,axis_z,angle)`' for a rotation of angle *angle* about axis ($axis\_x, axis\_y, axis\_z$), '`scale(x_factor,y_factor,z_factor)`' for scaling, '`translate(x_delta,y_delta,z_delta)`' for a translation and '`split(dir)`' for splitting the domain in half along direction '*dir*' ('*x*', '*y*' or '*z*'), which can be used to apply symmetries. For a 2D tessellation, the axis parameters can be omitted in '`rotate`' (default $(0, 0, 1)$), and the z component can be omitted in '`scale`' (default 1) and '`translate`' (default 0). An example is '`sphere(1,100):translate(-0.5,-0.5,-0.5):scale(0.5,1,2)`'.
Possible values: `see above`. Default value: `cube(1,1,1) in 3D and square(1,1) in 2D`.

`-periodicity` *char_string* [Option]

Specify the periodicity conditions that apply to the domain (and therefore to the tessellation). Provide as argument '`0`' (or '`none`') for no periodicity, '`1`' (or '`all`') for full periodicity, or a list of periodicity directions (among '`x`', '`y`' and '`z`') combined with '`,`' for semi-periodicity.
Possible values: `see above`. Default value: `0`.

Is it also possible to load a tessellation or a raster tessellation from a file,

`-loadtess` *file_name* [Input data]

Load a tessellation from a file. Provide as argument the file name.
Possible values: `any`. Default value: `none`.

`-loadtesr` *file_name* [Input data]

Load a raster tessellation from a file. Provide as argument the file name. To load only a region of a raster tessellation, use the syntax '*file_name*`:crop(`*xmin*`,`*xmax*`,`*ymin*`,`*ymax*`,`*zmin*`,`*zmax*`)`', where *xmin*, *xmax*, *ymin*, *ymax*, *zmin* and *zmax* are the minimum and maximum positions along *x*, *y* and *z*, respectively. For 2D raster tessellations, the *z* values can be omitted. To scale the number of voxels of a raster tessellation, use '*file_name*`:rasterscale(`*factor*`)`', where *factor* is the scaling factor, or '*file_name*`:scale(`*factor_x*`,`*factor_y*`,`*factor_z*`)`', where *factor_x*, *factor_y* and *factor_z* are the scaling factor along x, y and z, respectively. For 2D raster tessellations, the *z* value can be omitted.
Possible values: `any`. Default value: `none`.

Finally, it is possible to load a set of points. These points are used only for statistics, in option `-statpoint`; they are not seed points of the tessellation (see option `-morphooptiini` instead).

`-loadpoint` *file_name* [Input data]
Load points from a file. See Section B.4 [Position File], page 89, for the file format. Provide as argument the file name.
Possible values: `any`. Default value: `none`.

2.1.2 Morphology and Group Options

These options can be used to set the cell morphology. If you want to set seeds attributes instead, use '`-morphooptiini ... -morpho voronoi`'.

`-morpho` *char_string* [Option]
Specify morphological properties of the cells. It can be done either by using a special morphology string (as defined below), or by specifying custom cell properties such as sizes, sphericities, centroids, or even exact shapes (using a raster tessellation). Global properties (sometimes refered to as *morphological texture*) can be added. Alternatively, a tessellation can be loaded.
(i) The special morphology strings are the following (mutually-exclusive):
• '`voronoi`' for a standard Poisson-Voronoi tessellation;
• '`graingrowth`' or '`gg`' for grain-growth statistical properties, which correspond to a wider grain size distribution and higher grain sphericities than in a Voronoi tessellation (it actually is an alias for '`diameq:lognormal(1,0.35),1-sphericity:lognormal(0.145,0.03)`' in 3D and '`diameq:lognormal(1,0.42),1-circularity:lognormal(0.100,0.03)`' in 2D, see below); the '`graingrowth(`*`mean`*`)`' and '`gg(`*`mean`*`)`' variants can be used to provide an absolute mean grain size, *`mean`* (in which case `-n from_morpho` must be used, see below);
• '`centroidal`' for a centroidal tessellation[5] (it actually is an alias for '`centroid:seed`', see below);
• '`cube(`*`N`*`)`' / '`square(`*`N`*`)`' for a regular tessellation into cubic / square cells, where '*`N`*' is the number of cells along a direction, or '`cube(`*`N1,N2,N3`*`)`' / '`square(`*`N1,N2`*`)`' for a regular tessellation into cubic / square cells, where '*`N1`*', '*`N2`*' and '*`N3`*' are the number of cells along the three coordinate axes;
• '`tocta(`*`N`*`)`' for a regular tessellation into truncated octahedra, where '*`N`*' is the number of cells along a direction;
• '`lamellar(w=`*`w`*`,v=`*`v`*`,pos=`*`pos`*`)`' for a lamellar morphology. Argument '`w=`*`w`*' is mandatory, and arguments '`v=`*`v`*' and '`pos=`*`pos`*' are optional. Argument '`w=`*`w`*' enables the specification of the absolute lamella width *`w`*. For specifying several widths, combine them with '`:`'. Argument '`v=`*`v`*' allows one to specify the lamella plane normals *`v`*. For randomly-distributed normals taken from a uniform distribution, use '`random`' (the default). For a direction of space, use '`(`*`dir_x,dir_y,dir_z`*`)`', where (dir_x, dir_y, dir_z) is the direction. For a direction of the parent crystal, use '`crysdir(`*`crysdir_x,crysdir_y,crysdir_z`*`)`', where $(crysdir\_x, crysdir\_y, crysdir\_z)$ is the crystal direction. Argument '`pos=`*`pos`*' enables the specification of the position of the lamellae, *`pos`*. It can be '*`random`*' for a random position (the default) or '*`start`*' for the first lamella starting (full-width) from the start point of the domain (along direction *`dir`*). In the case of a multiscale tessellation, multiscale cell files can be provided as values of '*`w`*', '*`v`*', and '*`pos`*' (see Section B.3 [Multiscale Cell File], page 88). *(ii)* Custom morphological properties can be defined by providing as argument the cell property and its value, combined with '`:`'. The available properties are the following:
• '`size`' for the size (volume in 3D and area in 2D) and '`diameq`' for the equivalent diameter;
• '`sphericity`' for the sphericity and '`1-sphericity`' for 1 − the sphericity (or '`circularity`'

[5] `centroidal` is not recommended as it does not correspond to a morphological property *per se*; size and/or sphericity properties should be used instead.

and '`1-circularity`');[6][7]
• '`centroid`' for the centroid;
• '`centroidtol`' for the centroid with a tolerance (see below for the format; centroids with a tolerance more than 1000 times as high as the minimum tolerance are simply disregarded);
• '`centroidsize`' for combined centroid and size, and '`centroiddiameq`' for combined centroid and equivalent diameter;
• '`tesr`' for cells of a raster tessellation.
Size, diameq and sphericity (and their variants) can be defined by statistical distributions or on a per-cell basis, while centroid can be defined only on a per-cell basis. The list of available statistical distributions is provided in Section A.1 [Mathematical and Logical Expressions], page 65. If the number of cells is defined (see option `-n`), the size or diameq distribution is scaled to get the specified number of cells; otherwise (i.e., `-n from_morpho` is used), the number of cells is determined from the size or diameq distribution. An interval of possible values can also be provided using '`interval(`*`min`*`,`*`max`*`)`'. A unique value can be assigned to all cells using '*`value`*', where '*`value`*' is the value. Cell-by-cell values can be provided using '`file(`*`file_name`*`)`', where '*`file_name`*' is the name of the file containing the cell values (see Section B.4 [Position File], page 89, for '`centroid`'; add a tolerance to each position, as last column, for '`centroidtol`'). For '`centroid`', provide '`seed`' to get a centroidal tessellation. For '`tesr`', '*`file_name`*' is the name of the raster tessellation file. If `-n` is set to '`from_morpho`', the number of cells is set to the number of cells of the raster tessellation.
(iii) The global cell properties are the following (mutually-exclusive):
• '`columnar(`*`dir`*`)`' for a columnar morphology along coordinate axis '*`dir`*', where '*`dir`*' can be '`x`', '`y`' or '`z`';
• '`bamboo(`*`dir`*`)`' for a bamboo morphology along coordinate axis '*`dir`*', where '*`dir`*' can be '`x`', '`y`' or '`z`';
• '`aspratio(`*`r1`*`,`*`r2`*`,`*`r3`*`)`', where '*`r1`*', '*`r1`*' and '*`r3`*' represents relative length along the coordinate axes. For a 2D tessellation, '*`r3`*' can be omitted. When provided, other properties, such as the equivalent diameter or the sphericity (circularity, in 2D), are considered to apply to the cells as if they had no aspect ratio.
(iv) A tessellation can be loaded using '`file(`*`file_name`*`)`', where '*`file_name`*' is the name of the tessellation file.
To specify several properties, combine them with '`,`' (centroids and sizes/equivalent diameters should be seen as one property and specified with `centroidsize`/`centroiddiameq`).
Possible values: `any`. Default value: `voronoi`.

`-morphooptiini` *`char_string`* [Option]
Specify the initial positions and/or weights of the seeds. The general form of the argument is '`coo:`*`coo_char_string`*`,weight:`*`weight_char_string`*', but it is also possible to read the seeds of a tessellation file (provide its name as argument). Different values of '*`coo_char_string`*' and '*`weight_char_string`*' are available, depending on the value of option `-morpho`:
• '*`weight_char_string`*' can be a real value, any mathematical expression based on the variables listed in Section A.2 [Tessellation Keys], page 67, especially '`radeq`', '`diameq`', '`avradeq`' and '`avdiameq`', or '`file(`*`file_name`*`)`' to load values from a file (either a file containing the values or a tessellation file to read seed weights from). The default depends on the value of

[6] Terms '`sphericity`' and '`circularity`' apply to 3D and 2D, respectively, but can be used interchangeably. The sphericity of a polyhedron corresponds to the ratio of the surface area of the sphere of equivalent volume to the surface area of the polyhedron. Similarly, the circularity of a polygon corresponds to the ratio of the perimeter of the circle of equivalent surface area to the perimeter of the polygon.

[7] The reason behind the '`1-sphericity`' (or '`1-circularity`') variable is that, for a grain growth microstructure, 1 − the sphericity follows a lognormal distribution; see *R. Quey and L. Renversade, Optimal polyhedral description of 3D polycrystals: Method and application to statistical and synchrotron X-ray diffraction data, Comput. Methods Appl. Mech. Engrg., vol. 330, pp. 308-333, 2018.*

option '-morpho': for 'voronoi', it is '0', for a cell-size statistical distribution, it is 'avradeq', and for cell-based size values (including -morpho tesr) , it is 'radeq'.
• '*coo_char_string*' can be 'random' for random positions, 'packing' for positions set by (rough) dense sphere packing using the weights as sphere radii, 'centroid' for cell centroids, 'LLLFP2011' for Lyckegaard et al.'s method[8], or 'file(*file_name*)' to load values from a file (either a position file, See Section B.4 [Position File], page 89, or a tessellation file to read seed coordinates from). The default depends on the value of option '-morpho': for 'voronoi', it is 'random', for a cell-size statistical distribution, it is 'none', and for cell-based coordinate values (including -morpho tesr), it is 'centroid'.
Possible values: see above. Default value: default.

-morphooptiobjective *char_string* [Secondary option]
Specify the objective function. The argument should be of the form '*prop1*:*objective_function1*,*prop2*:*objective_function2*,...', where *propx* are properties as defined in option -morpho, and *objective_functionx* are their objective functions. An objective function depends on the property and its definition.
• For properties defined by a statistical distribution (which can be 'size', 'diameq', 'sphericity' or '1-sphericity' (or 'circularity' and '1-circularity')), the available values are 'chi2' (Chi-square test), 'ks' (Kolmogorov-Smirnov test), 'kuiper' (Kuiper's test), 'cmv' (Cramér-Von Mises test), 'ad' (Anderson-Darling test), 'FL2' (L^2-norm on F), 'FL2w' (weighted L^2-norm on F)[9], 'FL2wu' (weighted L^2-norm on F corresponding to 'FL2w' for a unimodal distribution), and the default value is 'FL2w'.
• For 'centroid', a Minkowski distance between the seeds and centroids is used, and can be 'L1', 'L2' or 'Linf'.
• For 'tesr', the definition of the objective function includes several factors. First, preprocessing operations to the raster tessellation can be applied using 'transform(*operations*)', where '*operations*' can include 'scale' to scale the tessellation to correct for a global cell elongation or 'rasterscale' to scale the raster itself to correct for a global voxel elongation (which may result from operation 'scale'); combine with ','. Second, control points can be defined using 'pts(*args*)' where 'args' can include 'region=*region*' where '*region*' can be 'surf' for surface voxels or 'all' for all voxels, and 'res=*res*' where '*res*' is the resolution, i.e. the average number of control points along a direction of a grain; combine with ','. Third, the expression of the objective function *per se* can be specified using 'val(*expr*)', where '*expr*' can be 'bounddist' for minimizing the distance between the raster tessellation and tessellation cell boundaries, or 'intervol' for maximizing the volume of intersection between the raster tessellation and tessellation (both provide similar results). To define the objective function, combine the above factors using '+'. The default value is 'pts(region=surf,res=5)+val(bounddist)'. It is finally possible to define how the different parts of the objective function are combined into the objective function (in the case where several properties are specified), using 'general:*objective_function*', where '*objective_function*' can be 'L1', 'L2' or 'Linf'; the default is 'L2'.
Possible values: any. Default value: default.

-morphooptidof *char_string* [Secondary option]
Specify the degrees of freedom. The available values are 'x', 'y' and 'z' for the 3 coordinates, and 'w' for the weights. Combine with ','.
Possible values: see above. Default value: x,y,z,w.

[8] A. Lyckegaard, E.M. Lauridsen, W. Ludwig, R.W. Fonda, and H.F. Poulsen. On the Use of Laguerre Tessellations for Representations of 3D Grain Structures. Advanced Engineering Materials, vol. 13, pp. 165–170, 2011.

[9] *R. Quey and L. Renversade, Optimal polyhedral description of 3D polycrystals: Method and application to statistical and synchrotron X-ray diffraction data, Comput. Methods Appl. Mech. Engrg., vol. 330, pp. 308-333, 2018.*

`-morphooptistop` *char_string* [Secondary option]
Specify the stopping criteria of the optimization process. Not all criteria need to be defined; in most cases, only one or two are needed. A stopping expression must be of the form '*var=val*', where '*var*' is a variable and '*val*' is its value. The available variables are: an absolute or relative error on the value of the objective function evaluated on a number of degrees of freedom basis, '*eps*' or '*reps*' (use '*nlopt_eps*' or '*nlopt_reps*' for the NLopt iteration-based values), an absolute or relative error on the components of the solution vector, '*xeps*' or '*xreps*', a value of the objective function, '*val*', a maximum number of iterations, '*itermax*', a maximum computation time, '*time*', or a maximum number of iteration loops, '*loopmax*' (see option `-morphooptialgomaxiter`). Combine them with '`,`'. Optimization stops as soon as one stopping criterion is verified. Optimization can also be stopped anytime using the Ctrl+C command.
Possible values: `any`. Default value: `eps=1e-6 (val=1e-4,iter=10000 for -morpho centroidal)`.

`-morphooptialgo` *char_string* [Secondary option]
Specify the optimization algorithm. The available values are '`subplex`' (Subplex), '`praxis`' (Praxis), '`neldermead`' (Nelder-Mead), '`cobyla`' (Cobyla), '`bobyqa`' (Bobyqa) and '`newuoa`' (Newuoa) — only '`subplex`' and '`praxis`' are recommended; it is also possible to provide several algorithms combined with '`,`', in which case the additional algorithms may be used if previous ones fail. In the case of `-morpho centroidal`, another available value is '`lloyd`' (Lloyd's algorithm); to specify the seed displacement factor (from the seed to the centroid), use '`lloyd(`*factor*`)`' (the default value is 1.9). Another available value (use only if you know what you are doing) is '`random(`*seednb*`,`*dimnb*`,`*min*`,`*max*`,`*id*`)`', for which, at each odd iteration, each of '*seednb*' seeds sees '*dimnb*' of its attributes (among those specified by option `-morphooptidof`) being randomly perturbed, the norm of the total perturbation vector ranging from '*min*'–'*max*'; '*id*' is the identifier of the distribution (similarly to option `-id`); variables can be any mathematical expression based on '*seednb*' (the total number of seeds), '*dim*' (the tessellation dimension), '*avdiameq*' (the average equivalent cell diameter) and '*inistep*' (the value of `-morphooptiinistep`); at each next (even) iteration, the attributes of the seeds are reverted to their original values.
Possible values: `any`. Default value: `subplex,praxis (lloyd for -morpho centroidal)`.

`-morphooptigrid` *char_string* [Secondary option]
Specify the grids used to discretize the distributions. Provide the values using '*var*`:`*grid*', where *var* is the variable, among `diameq`, `size`, `sphericity` and `1-sphericity` (or `circularity` and `1-circularity`), and *grid* is the grid. The grid must be of the form '`regular(`*min*`,`*max*`,`*bin_nb*`)`', where *min* and *max* are the minimum and maximum values of the grid interval, respectively, and *bin_nb* is the number of bins.
Possible values: `any`. Default value: `diameq:regular(-1,10,1100),size:regular(-1,10,1100),sphericity:regular(-0.1,1.1,1200),1-sphericity:regular(-0.1,1.1,1200)`.

`-morphooptismooth` *char_string* [Secondary option]
Specify the standard deviations of the Gaussian distributions which are assigned to each cell data to compute the distributions. Provide the values using '*var*`:`*val*', where *var* is the variable, among `diameq`, `size`, `sphericity` and `1-sphericity` (or `circularity` and `1-circularity`), and *val* is the value. It is also possible to specify how the convolution functions should be treated: provide '`analytical`' for analytical functions or '`numerical`' for numerical functions (the default, recommended). Combine with '`,`'.
Possible values: `any`. Default value: `diameq:0.05,size:0.05,sphericity:0.005,numerical`.

`-morphooptideltamax` *real* [Secondary option]
Specify the maximal value by which each variable is allowed to change during optimization. Possible values: `any>=0`. Default value: `HUGE_VAL`.

`-morphooptiinistep` *real* [Secondary option]
Specify the step used to perturb the seed positions and weights when optimization begins. The argument can be a function of *avdiameq*, the average equivalent cell diameter. Possible values: `any>0`. Default value: `avdiameq/10`.

`-morphooptilogtime` *char_string* [Secondary option]
Log the time taken during the optimization process. The keys are provided in Section A.4 [Tessellation Optimization Keys], page 71. The log file has extension `.logtime`. Possible values: `any`. Default value: `none`.

`-morphooptilogvar` *char_string* [Secondary option]
Log the variables (seed attributes) during the optimization process. The keys are provided in Section A.4 [Tessellation Optimization Keys], page 71. The log file has extension `.logvar`. Possible values: `any`. Default value: `none`.

`-morphooptilogval` *char_string* [Secondary option]
Log the value of the objective function during the optimization process. The keys are provided in Section A.4 [Tessellation Optimization Keys], page 71. The log file has extension `.logval`. Possible values: `any`. Default value: `none`.

`-morphooptilogdis` *char_string* [Secondary option]
Log the distributions during the optimization process. The keys are provided in Section A.4 [Tessellation Optimization Keys], page 71. The log files have extension `.logdis*`. Possible values: `any`. Default value: `none`.

`-morphooptilogtesr` *char_string* [Secondary option]
Log the raster tessellation voxel data during the optimization process. The keys are provided in Section A.4 [Tessellation Optimization Keys], page 71. The log file has extension `.logtesr`. Possible values: `any`. Default value: `none`.

`-morphooptialgomaxiter` *real* [Secondary option]
Specify the maximum number of iterations allowed to the optimization algorithm to run without decreasing the objective function. The expression can be any mathematical expression based on variable '*varnb*' (the total number of optimization variables). Possible values: `any`. Default value: `max(varnb,1000)`.

These options can be used to define cell groups (each cell is assigned to a group). Groups are defined after tessellation and so can be defined from the cell properties.

`-group` *char_string* [Option]
Specify the groups of the cells. Provide an expression based on the variables defined in Section A.2 [Tessellation Keys], page 67, or '`file(`*file_name*`)`' to load values from a file. Possible values: `any`. Default value: `none`.

2.1.3 Crystal Orientation Options

`-ori` *char_string* [Option]
Specify the type of crystal orientation distribution. It can be:
- '`random`' for randomly-distributed orientations in 3D space;
- '`uniform`' for uniformly-distributed orientations in 3D space (the crystal symmetry must be specified using `-oricrysym`);

• '`fibre(dirs_x,dirs_y,dirs_z,dirc_x,dirc_y,dirc_z)`' for randomly-distributed orientations about the fibre defined by crystal direction (*dirc_x*, *dirc_y*, *dirc_z*) parallel to sample direction (*dirs_x*, *dirs_y*, *dirs_z*);
• an ideal orientation, (see Section A.9 [Rotations and Orientations], page 75);
• a discrete orientation defined using an orientation descriptor (see Section A.9 [Rotations and Orientations], page 75);
• '`equal`' for orientations equal to the one of the parent cell;
• '`spread(thetam)`' for orientations randomly distributed about the one of the parent cell, according to a 3-variate normal distribution so that the average misorientation angle with respect to the average orientation is equal to *thetam* (expressed in degree);
• '`file(filename,des=des)`' for orientations to be read from file *filename* and written using the descriptor *des* (see Section A.9 [Rotations and Orientations], page 75); if Rodrigues vector (`rodrigues`), the descriptor can be omitted.
Possible values: `see above`. Default value: `random`.

`-oridistrib` *char_string* [Option]
Specify the type of (in-cell) orientation distribution. It can be '`none`' for none or '`normal(thetam)`' for a 3-variate normal distribution so that the average misorientation angle (with respect to the average orientation) is equal to *thetam* (expressed in degree), or '`file(file_name)`' to load values from a file.
Possible values: `see above`. Default value: `none`.

`-oricrysym` *char_string* [Option]
Specify the crystal symmetry (see Section A.10 [Crystal Symmetries], page 76). This is used by option `-ori uniform` and to reduce the domain of definition of the orientation descriptors.
Possible values: `see above`. Default value: `triclinic`.

`-orioptiini` *char_string* [Secondary option]
Specify the initial crystal orientations. Provide '`random`' for random orientations, or '`file(filename,des=des)`' for reading orientations from file *filename* and written using the descriptor *des* (see Section A.9 [Rotations and Orientations], page 75); if Rodrigues vector (`rodrigues`), the descriptor can be omitted.
Possible values: `any`. Default value: `random`.

`-orioptifix` *char_string* [Secondary option]
Fix some orientations during optimization. Provide '`none`' for none, or '`file(filename)`', where *filename* contains a logical value for each orientation: '`0`' if the orientation is not fixed and '`1`' if the orientation is fixed.
Possible values: `any`. Default value: `none`.

`-orioptistop` *char_string* [Secondary option]
Specify the stopping criterion of the optimization process, under the form of a logical expression based on the following variables: the relative error on the forces at orientations, '*reps*', and the iteration number, '*iter*'.
Possible values: `any`. Default value: `reps<1e-3||iter>=1e3`.

`-orioptineigh` *char_string* [Secondary option]
Use only the close neighborhood of orientations to compute their forces (for '`-ori uniform`'). Specify the radius of the neighborhood, which can be any mathematical expression based on *dr* (the average radius of an orientation). *Nstar* is the grand number of orientations (i.e., taking crystal symmetry into account).
Possible values: `any`. Default value: `Nstar<10000?pi:20*dr`.

`-orioptilogvar` *char_string* [Secondary option]
Log the variables (the orientations) during the optimization process. The keys are provided in Section A.5 [Orientation Optimization Keys], page 73. The log file has extension `.logorivar`. Possible values: `any`. Default value: `none`.

2.1.4 Transformation Options

`-transform` *char_string(...)* [Option]
Apply transformations to a tessellation (if scalar and raster tessellations are written in output, they are transformed independently; i.e., rasterization preceeds transformation).

The following transformations apply to a scalar tessellation:
• '`scale(`*x_fact*`,`*y_fact*`,`*z_fact*`)`' scales a tessellation by *x_fact*, *y_fact* and *z_fact* along directions x, y and z, respectively. For a 2D tessellation, *z_fact* can be omitted.
• '`rotate(`*axis_x*`,`*axis_y*`,`*axis_z*`,`*angle*`)`' for a rotation about the centre and by an axis/angle pair.[10]
• '`translate(`*dist_x*`,`*dist_y*`,`*dist_z*`)`' for a translation by distances *dist_x*, *dist_y* and *dist_z* along directions x, y and z, respectively.
• '`cut(`*primitive1*`,`*primitive2*`,...)`' for cutting by a series of geometrical primitives (experimental). The primitives can be:
(i) '`hspace(d,a,b,c)`' for the half-space of equation $a\,x + b\,y + c\,z \geq d$;
(ii) '`sphere(`*centre_x*`,`*centre_y*`,`*centre_z*`,`*rad*`)`' for a sphere of centre (*centre_x*, *centre_y*, *centre_z*) and radius *rad*;
(iii) '`cylinder(`*basis_x*`,`*basis_y*`,`*basis_z*`,`*axis_x*`,`*axis_y*`,`*axis_z*`,`*rad*`)`' for a cylinder of basis point (*basis_x*, *basis_y*, *basis_z*), axis (*axis_x*, *axis_y*, *axis_z*) and radius *rad*;
(iv) '`ecylinder(`*basis_x*`,`*basis_y*`,`*basis_z*`,`*axis_x*`,`*axis_y*`,`*axis_z*`,`*esaxis1_x*`,`*esaxis1_y*`,`*esaxis1_z*`,`*esaxis2_x*`,`*esaxis2_y*`,`*esaxis2_z*`,`*srad1*`,`*srad2*`)`' for an elliptic cylinder of basis point (*basis_x*, *basis_y*, *basis_z*), axis (*axis_x*, *axis_y*, *axis_z*), ellipse section first axis (*esaxis1_x*, *esaxis1_y*, *esaxis1_z*), ellipse section second axis (*esaxis2_x*, *esaxis2_y*, *esaxis2_z*), ellipse section first radius *esrad1* and ellipse section second radius *esrad2*.
Append '`i`' to a primitive name (to get '`cylinderi`', etc.) for the complementary shape.
• '`planecut(d,a,b,c)`' for cutting by the (oriented) plane of equation $a\,x + b\,y + c\,z = d$.
• '`crop(`*primitive*`)`' crops the tessellation by a primitive. The primitive can be:
(i) '`cube(`*xmin*`,`*xmax*`,`*ymin*`,`*ymax*`,`*zmin*`,`*zmax*`)`' for a cube defined by its x, y and z bounds.
• '`slice(d,a,b,c)`' for slicing a 3D tessellation by the (oriented) plane of equation $a\,x + b\,y + c\,z = d$ (yielding to a 2D tessellation).
• '`mergecell(`*expr1*`,`*expr2*`,...)`' for merging cells matching expression *expr1*, *expr2*, etc., where expressions are based on the variables defined in Section A.2 [Tessellation Keys], page 67. Cell merging operates incrementally through expressions.
• '`rmcell(`*expr1*`,`*expr2*`,...)`' for removing cells matching expression *expr1*, *expr2*, etc., where expressions are based on the variables defined in Section A.2 [Tessellation Keys], page 67. Cell removing operates incrementally through expressions.
• '`resetcellid`' for resetting cell ids (contiguous numbering from 1).

The following transformations apply to a raster tessellation:
• '`scale(`*x_fact*`,`*y_fact*`,`*z_fact*`)`' scales a tessellation by *x_fact*, *y_fact* and *z_fact* along directions x, y and z, respectively. For a 2D tessellation, *z_fact* can be omitted.
• '`rotate(`*axis_x*`,`*axis_y*`,`*axis_z*`,`*angle*`)`' for a rotation about the centre and by an axis/angle pair.
• '`translate(`*dist_x*`,`*dist_y*`,`*dist_z*`)`' for a translation by distances *dist_x*, *dist_y* and *dist_z* along directions x, y and z, respectively.

[10] Cell orientations are rotated accordingly.

• '`renumber`' renumbers a tessellation to remove cells that are empty or have a zero id.
• '`unindex`' assigns a zero cell id to voxels of orientation (0, 0, 0) (in Rodrigues vector).
• '`oriaverage`' sets the cell orientations (field '`**cell/*ori`') as the averages of the cell voxel orientations (field '`**oridata`').
• '`crop(primitive)`' crops the raster tessellation by a primitive. The primitive can be:
(i) '`cube(xmin,xmax,ymin,ymax,zmin,zmax)`' for a cube defined by its x, y and z bounds;
(ii) '`cylinder(centre_x,centre_y,diameter)`' for a cylinder of z axis.
• '`autocrop`' reduces the raster to its minimal size.
• '`rasterscale(x_fact,y_fact,z_fact)`' scales the number of voxels of the raster by factors *x_fact*, *y_fact* and *z_fact* along directions x, y and z, respectively. For a 2D tessellation, *z_fact* can be omitted.
• '`rmsat`' removes the cell "satellites", i.e. parts disconnected from the cell bulk.
• '`grow`' grows the cells to fill the domain.
• '`tessinter(tess_file)`' computes the intersection with tessellation *tess_file*.
• '`addbuffer(buffx,buffy,buffz)`' adds a buffer of *buffx* void voxels on both sides in the x direction, a buffer of *buffy* void voxels on both sides in the y direction and a buffer of *buffz* void voxels on both sides in the z direction.
• '`2d`' transforms a 3D tessellation with 1 voxel along z into a 2D tessellation.
Several transformations can be applied successively by combining them with '`,`'.
Possible values: `any`. Default value: `none`.

`-sort` *char_string* [Secondary option]
Sort the tessellation cells (typically to facilitate data post-processing). Provide as argument the mathematical expression used for sorting (see Section A.1 [Mathematical and Logical Expressions], page 65).
Possible values: `any`. Default value: `none`.

2.1.5 Regularization Options

`-regularization` *logical* [Option]
Regularize a tessellation, that is, removes the small edges and, indirectly, the small faces. This is controlled by options `-fmax`, `-sel` and `-mloop`. Regularization enables meshing with higer-quality elements using module -M (see Chapter 3 [Meshing Module (-M)], page 29), at the cost that some internal faces (of a 3D tessellation) can become slightly non-planar.
Possible values: `0 or 1`. Default value: `0`.

`-fmax` *real* [Option]
Specify the maximum allowed face flatness fault (in degrees). The flatness fault is the maximum angle between the normals at two locations on a face.
Possible values: `0 to 180`. Default value: `20`.

`-sel or -rsel` *real* [Secondary option]
Specify the absolute or relative small edge (maximum) length. `rsel` is defined relative to the average cell size (volume in 3D and area in 2D). The default `-rsel 1` leads to a length of 0.25 for a unit volume cell in 3D and 0.125 for a unit area cell in 2D. The value also allows one to avoid mesh refinement with the default meshing parameters (see Chapter 3 [Meshing Module (-M)], page 29). It is also possible to specify values on a per-cell basis. The first way is to use *default_sel,cell_expr1:cell_sel1,cell_expr2:cell_sel2...*, where *default_sel* is the default small edge length, *cell_expri* is an expression defining the set of cells *i* and *cell_seli* is the corresponding small edge length. '*cell_expri*' can be any expression based on variables provided in Section A.2 [Tessellation Keys], page 67. The expressions are processed one after the other. When processing expression *cell_expri*, the matching cells are assigned *cell_seli* as small edge length. Typically, option `-rsel` should be passed

the same argument than option `-rcl` of module -M, see Chapter 3 [Meshing Module (-M)], page 29. The second way is to load values from an external file using '`file(`*`file_name`*`)`', where *`file_name`* is the name of the file containing the length values.
Possible values: `any`. Default value: `-rsel 1`.

`-mloop` *`integer`* [Secondary option]
Specify the maximum number of regularization loops. During each loop, the small edges are considered for removal in turn from the shortest to the longest. Regularization stops when the maximum number of loops is reached or no edges are deleted during a loop.
Possible values: `any`. Default value: `2`.

2.1.6 Output Options

`-o` *`file_name`* [Option]
Specify the output file name.
Possible values: `any`. Default value: `none`.

`-format` *`char_string`* [Option]
Specify the format of the output file(s). For scalar tessellations, the available formats are the Neper '`tess`', the Gmsh '`geo`', the Ply '`ply`', the STL '`stl`' (for a separate file for each cell, append '`:bycell`)', the Wavefront '`obj`', the 3dec '`3dec`' and the Surface Evolver '`fe`'. For raster tessellations, the available formats are the Neper '`tesr`', the Orilib map format '`olmap`', and the VTK format '`vtk`'. Orientations for the cells can be obtained using '`ori`' (see also options beginning with '`-ori`'). Combine the values with '`,`'.
Possible values: `see above`. Default value: `tess`.

`-tesrformat` *`char_string`* [Option]
Specify the format of the raster output file(s). The available formats are ASCII ('`ascii`'), 8-bit binary / unsigned char-type ('`binary8`'), 16-bit binary / short-type ('`binary16`' and '`binary16_big`') and 32-bit binary / int-type ('`binary32`' and '`binary32_big`'). Formats '`binary16`' and '`binary32`' mean little endianness while formats '`binary16_big`' and '`binary32_big`' mean big endianness.[11]
Possible values: `see above`. Default value: `binary16 or binary_big (depending on the system)`.

`-tesrsize` *`integer`* [Option]
Specify the number of points of a raster tessellation along a direction of the domain. In case of a domain of different lengths along the different directions, the argument stands for the geometrical average of the number of points along the different directions, so that the raster points are as close to cubic as possible. To specify different values along the x, y and z directions, combine the values with '`:`'.
Possible values: `any`. Default value: `20`.

`-oridescriptor` *`char_string[:char_string]`* [Option]
Specify the orientation descriptor and (optionally) the orientation convention used in the `.tess`, `.tesr` and `.ori` files, under the form *`descriptor:convention`*. The descriptor can be Rodrigues vector, (`rodrigues`), Euler angles in Bunge, Kocks or Roe convention (`euler-bunge`, `euler-kocks`, `euler-roe`), rotation matrix (`rotmat`), axis / angle of rotation (`axis-angle`), angle of rotation (`angle`), or quaternion (`quaternion`). The convention can be `active` or `passive`, and is `active` by default.
Possible values: `see above`. Default value: `rodrigues`.

[11] Endianness is both written in the tesr file and tested on the system when reading the tesr file, so that the user normally does not have to care about it (even when transferring files across systems).

`-oriformat` *char_string* [Option]
Specify the format(s) of the `.ori` output file(s). The available formats are: `plain` (i.e. only the descriptors on successive lines) and the Z-set `geof`[12]. Combine with '`,`'. If several formats are requested, the format is appended to the file name as in '*`filename`*`.ori-plain`' and '*`filename`*`.ori-geof`'.
Possible values: `see above`. Default value: `plain`.

2.1.7 Post-Processing Options

The following two options provide general statistics on tessellations,

`-stattess` *char_string* [Post-processing]
Provide statistics on the tessellation. Give as argument the keys as described in Section A.2 [Tessellation Keys], page 67, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.sttess`.

`-stattesr` *char_string* [Post-processing]
Provide statistics on the raster tessellation. Give as argument the keys as described in Section A.3 [Raster Tessellation Keys], page 70, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.sttesr`.

The next options apply to the cells and seeds of a tessellation or a raster tessellation, independently of its dimension,

`-statcell` *char_string* [Post-processing]
Provide statistics on the tessellation cells. Give as argument the keys as described in Section A.2 [Tessellation Keys], page 67, for a tessellation and Section A.3 [Raster Tessellation Keys], page 70, for a raster tessellation, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stcell`.

`-statseed` *char_string* [Post-processing]
Provide statistics on the tessellation seeds. Give as argument the keys as described in Section A.2 [Tessellation Keys], page 67, for a tessellation and Section A.3 [Raster Tessellation Keys], page 70, for a raster tessellation, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stseed`.

For a tessellation, it is also possible to get statistics on an per-entity basis,

`-statver` *char_string* [Post-processing]
Provide statistics on the tessellation vertices. Give as argument the keys as described in Section A.2 [Tessellation Keys], page 67, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stver`.

`-statedge` *char_string* [Post-processing]
Provide statistics on the tessellation edges. Give as argument the keys as described in Section A.2 [Tessellation Keys], page 67, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stedge`.

[12] Euler angles in Bunge convention are written.

`-statface` *char_string* [Post-processing]
Provide statistics on the tessellation faces. Give as argument the keys as described in Section A.2 [Tessellation Keys], page 67, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stface`.

`-statpoly` *char_string* [Post-processing]
Provide statistics on the tessellation polyhedra. Give as argument the keys as described in Section A.2 [Tessellation Keys], page 67, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stpoly`.

For a raster tessellation, it is also possible to get statistics on an per-voxel basis,

`-statvox` *char_string* [Post-processing]
Provide statistics on the tessellation voxels. Give as argument the keys as described in Section A.3 [Raster Tessellation Keys], page 70, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stpoly`.

Finally, it is possible to get statistics for a particular set of points.

`-statpoint` *char_string* [Post-processing]
Provide statistics on points. The points must be loaded with option `-loadpoint`. Give as argument the keys as described in Section A.7 [Point Keys], page 74, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stpoint`.

2.1.8 Debugging Options

`-checktess` *file_name* [Input data]
Check a tessellation file. Provide as argument the file name. Use this option if the tessellation file fails to load using option `-loadtess` or in other modules.
Possible values: `any`. Default value: `none`.

2.2 Output Files

2.2.1 Tessellation

- Neper tessellation file: `.tess`

  It contains a scalar description of the tessellation. See Section B.1 [Tessellation File (`.tess`)], page 81, for details.
- Neper raster tessellation file: `.tesr`

  It contains a raster description of the tessellation. See Section B.2 [Raster Tessellation File (`.tesr`)], page 86, for details.
- Orilib map file: `.olmap`

  It contains a description of a 2D raster tessellation as an orientation map and written under the Orilib format `.olmap`.
- Gmsh geometry file: `.geo`

  It contains a minimal description of the tessellation written under the Gmsh geometry file format `.geo`. This file can be opened with Gmsh for interactive visualization.
- Ply file: `.ply`

  It contains a description of the tessellation written under the standard "Polygon File Format" `.ply`.

- STL file: `.stl`

  It contains a description of the tessellation written under the STL (STereoLithography) format `.stl`. If '`-format stl:bycell`' is used, a separate file is written for each cell, whose name ends in `-id.stl`, where '*id*' is the cell identifier written with leading zeros.
- Wavefront geometry file: `.obj`

  It contains a description of the tessellation written under the Wavefront geometry format `.obj`.
- 3dec file: `.3dec`

  It contains a description of the tessellation written under the 3dec format `.3dec`.
- VTK file: `.vtk`

  It contains a description of the raster tessellation written under the VTK format `.vtk` as supported by Amitex_ffpt. Binary data are always written using big endians.
- Orientation file: `.ori`

  It contains crystal orientations for the tessellation cells. The orientations are written on successive lines, using the descriptor specified by option `-oridescriptor` (see also Section A.9 [Rotations and Orientations], page 75) and the writing convention specified by option `-oriformat`.

2.2.2 Statistics

Statistics files are first provided for the tessellation and raster tessellation. Each file contains the data specified to the corresponding `-stat` option and as described in Section A.2 [Tessellation Keys], page 67, and Section A.3 [Raster Tessellation Keys], page 70.

- Tessellation statistics file, `.sttess`.
- Raster tessellation statistics file, `.sttesr`.

Statistics files are also provided for cells, seeds, vertices, edges, faces, polyhedra and points. They are formatted with one line per entity. Each line contains the data specified to the corresponding `-stat` option and described in Section A.2 [Tessellation Keys], page 67, and Section A.3 [Raster Tessellation Keys], page 70.

- Tessellation cell statistics file, `.stcell`.
- Tessellation seed statistics file, `.stseed`.
- Tessellation vertex statistics file, `.stver`.
- Tessellation edge statistics file, `.stedge`.
- Tessellation face statistics file, `.stface`.
- Tessellation polyhedron statistics file, `.stpoly`.
- Point statistics file, `.stpoint`.

2.2.3 Tessellation Optimization Log Files

Log files are provided for the time, variables, statistical distributions and objective function value. The files contain the data specified to the corresponding `-morphooptilog` option and described in Section A.4 [Tessellation Optimization Keys], page 71.

- Time file, `.logtime`.
- Variables (seed attributes) file, `.logvar`.
- Statistical distribution files, `.logdisid`, where *id* is the identifier of the distribution.
- Objective function value file, `.logval`.
- Target raster tessellation file, `-obj.tesr`.

2.2.4 Orientation Optimization Log Files

A log file is provided for the orientation variables. The files contain the data specified to the `-orioptilogvar` option and described in Section A.5 [Orientation Optimization Keys], page 73.

- Variables (orientations) file, `.logorivar`.

2.3 Examples

Below are some examples of use of neper -T.

1. Generate a Voronoi tessellation containing 100 cells.
   ```
   $ neper -T -n 100
   ```
2. Generate a different Voronoi tessellation containing 100 cells (identifier = 2).
   ```
   $ neper -T -n 100 -id 2
   ```
3. Use an elongated domain and generate a Voronoi tessellation containing 100 cells.
   ```
   $ neper -T -n 100 -domain "cube(3,1,0.33)"
   ```
4. Generate a Voronoi tessellation containing 100 cells and apply regularization.
   ```
   $ neper -T -n 100 -reg 1
   ```
5. Generate a 2D Voronoi tessellation containing 100 cells.
   ```
   $ neper -T -n 100 -dim 2
   ```
6. Generate a tessellation containing 100 cells with an x columnar axis.
   ```
   $ neper -T -n 100 -morpho "columnar(x)"
   ```
7. Generate a tessellation containing 100 cells with a bamboo structure along x.
   ```
   $ neper -T -n 100 -morpho "bamboo(x)"
   ```
8. Generate a tessellation containing 100 cells with experimental grain-growth morphological properties.
   ```
   $ neper -T -n 100 -morpho gg
   ```
9. Generate a tessellation containing 100 cells with experimental grain-growth morphological properties and define groups by splitting cells based on their ids.
   ```
   $ neper -T -n 100 -morpho gg -group "id<=50?1:2"
   ```
10. Generate a tessellation containing 100 cells with experimental grain-growth morphological properties and an aspect ratio of 2:1:0.5.
    ```
    $ neper -T -n 100 -morpho "gg,aspratio(2,1,0.5)"
    ```
11. Generate a tessellation containing 100 cells with experimental grain-growth morphological properties, and get the equivalent diameters and sphericities of the cells.
    ```
    $ neper -T -n 100 -morpho gg -statcell diameq,sphericity
    ```
12. Generate a tessellation of specified absolute grain size distribution (the number of cells is determined accordingly).
    ```
    $ neper -T -n from_morpho -morpho
      "diameq:lognormal(0.1,0.03),1-sphericity:lognormal(0.145,0.03)"
    ```
13. Generate a tessellation in a non-convex domain (by cutting the tessellation once generated).
    ```
    $ neper -T -n 100 -morpho gg
      -transform "cut(cylinder(1.2,0.5,0.5,0,1,0,0.4))"
    ```
14. Generate a 2-scale Voronoi tessellation containing 100×10 cells.
    ```
    $ neper -T -n 100::10
    ```
15. Generate a 2-scale Voronoi tessellation containing 100×10 cells, with different tessellations at scale 2 (identifier = 2) (identifier = 2).
    ```
    $ neper -T -n 100::10 -id 1::2
    ```

16. Generate a 2-scale tessellation containing 10 primary cells with grain-growth morphological properties, each one divided into lamellae of width 0.1.

```
$ neper -T -n 10::from_morpho -morpho "gg::lamellar(w=0.1)"
```

17. Generate a 2-scale Voronoi tessellation containing 10 primary cells with grain-growth morphological properties, each one divided into lamellae of widths loaded from file `lam_width` and plane normals loaded from file `lam_normal`.

```
$ neper -T -n 10::from_morpho -morpho "gg::lamellar(w=msfile(lam_
width),v=msfile(lam_normal))"
```

```
lam_width:
 1 0.05
 2 0.10
 3 0.05
 4 0.10
 5 0.05
 6 0.10
 7 0.05
 8 0.10
 9 0.05
10 0.10
```

```
lam_normal:
 1 1.000000 0.000000 0.000000
 2 0.000000 1.000000 0.000000
 3 1.000000 0.000000 0.000000
 4 0.000000 1.000000 0.000000
 5 1.000000 0.000000 0.000000
 6 0.000000 1.000000 0.000000
 7 1.000000 0.000000 0.000000
 8 0.000000 1.000000 0.000000
 9 1.000000 0.000000 0.000000
10 0.000000 1.000000 0.000000
```

18. Generate a 2-scale Voronoi tessellation containing 3 primary cells divided into 1, 10 and 100 secondary cells, respectively.

```
$ neper -T -n "3::msfile(myfile)" -id 1::1
```

```
myfile:
1 1
2 10
3 100
```

19. Generate a 2-scale Voronoi tessellation containing 2×3 cells with specific seed coordinates at both scales (files `coo1` and `coo2`).

```
$ neper -T -n 2::3 -id 1::1 \
  -morphooptiini "coo:file(coo1),weight:0::coo:msfile(coo2),weight:0" \
  -morpho voronoi
```

```
coo1:
0.25 0.50 0.50
0.75 0.50 0.50
coo2:
1 0.25 0.10 0.50
1 0.25 0.50 0.50
1 0.25 0.90 0.50
2 0.75 0.50 0.10
```

```
2 0.75 0.50 0.50
2 0.75 0.50 0.90
```

Note that `coo1` is a simple position file (see Section B.4 [Position File], page 89) while `coo2` is a multiscale cell file (see Section B.3 [Multiscale Cell File], page 88).

20. Generate a Voronoi tessellation containing 100 cells with uniformly distributed crystal orientations and cubic crystal symmetry.

    ```
    $ neper -T -n 100 -oricrysym cubic -ori uniform
    ```

21. Generate 100 uniformly distributed crystal orientations with cubic crystal symmetry (no tessellation).

    ```
    $ neper -T -n 100 -oricrysym cubic -ori uniform -for ori
    ```

3 Meshing Module (-M)

Module -M is the module for meshing scalar and raster tessellations. Two meshing strategies are available. *Free (or unstructured) meshing* creates a conforming mesh into tetrahedral elements (triangular in 2D). *Mapped (or structured) meshing* generates a non-conforming mesh into regular hexahedral elements (quadrangular in 2D). Free meshing is carried out so that the elements have sizes as close as possible to the target value, and show high quality, that is, with shapes as close to equilateral as possible. The input file is a tessellation file (`.tess`) or a raster tessellation file (`.tesr`), as provided by module -T. Standard tessellations, multiscale tessellations, and periodic (or semi-periodic) tessellations are supported. Free meshing of raster tessellations works for 2D tessellations only. The output mesh can be written in written at the msh format, which can be readily used by FEPX, or other formats.

The target element size of the mesh can be specified through the element *characteristic length (*`cl`*')*. It corresponds to the length of a 1D element, the length of the edge of a triangular or quadrangular element (2D), and the length of an edge of a tetrahedral or hexahedral element (3D). For convenience, a *relative characteristic length (*`rcl`*)* is also defined, whose value is relative to the average cell size and provides a medium number of elements. It is also possible to specify `cl` (or `rcl`) values on a per-cell basis, or to specify different values along x, y and z.

For free meshing, mesh quality is ensured to the greatest extent possible using several advanced capabilities,[1]

- Optimized meshing rules. The mesh properties are controlled by size parameters (options `-cl`, `-rcl`, etc.) and a size gradient parameter used for 1D meshing (option `-pl`).
- Multimeshing. Each tessellation face and volume is meshed separately of the others, with several meshing algorithms, until a target mesh quality is reached. This is controlled by options beginning with `-meshqual`, and options `-mesh2dalgo` and `-mesh3dalgo`.

Note that, in general, tessellation *regularization* is also necessary to ensure good-quality meshing, see Chapter 2 [Tessellation Module (-T)], page 11.

Remeshing can also be applied to generate a new, good-quality mesh from a mesh containing poor-quality elements. The variables defined on the parent mesh can be transported on the child mesh (options beginning with `-transport`).

For mapped meshing, mesh cleaning options enable the removal of isolated elements or duplicate nodes, or to duplicate nodes subjected to singularity behavior (options `-clean`, `-dupnodemerge` and `-singnodedup`).

Mesh partitioning allows for the division the mesh nodes and elements into several sets while minimizing the interfaces between them[2], for parallel finite element calculations. It is mandatory for parallel simulations with FEPX. Partitioning can return any number of partitions or, more efficiently, can be carried out according to a given parallel computer architecture (options beginning with `-part`).

In the output mesh, the individual entities of the tessellations (the vertices, edges, faces and polyhedra) can be described by element sets (option `-dim`). Node sets of the vertices, edges and faces of the boundary of the tessellation are also provided for prescribing the boundary conditions (option `-nset`). The surface element sets are also provided (option `-faset`). Element sets other than those corresponding to the tessellation cells can be defined (option `-elset`). The mesh order can be 1 or 2 (option `-order`). Statistical data can be obtained on the meshes (options beginning with `-stat`).

---

[1] See *R. Quey, P.R. Dawson and F. Barbe, Large-scale 3D random polycrystals for the finite element method: Generation, meshing and remeshing, Comput. Methods Appl. Mech. Engrg., vol. 200, pp. 1729-1745, 2011.*

[2] Each partition being assigned to a computation core in the finite element calculation, the minimization of the interfaces between the partitions is done in terms of the number of necessary communications between computation cores.

Here is what a typical run of module -M looks like:

```
$ neper -M n10-id1.tess

=======================    N   e   p   e   r    ======================
Info   : A software package for polycrystal generation and meshing.
Info   : Version 4.0.0
Info   : Built with: gsl|muparser|opengjk|openmp|nlopt|libscotch (full)
Info   : Running on 8 threads.
Info   : <http://neper.info>
Info   : Copyright (C) 2003-2020, and GNU GPL'd, by Romain Quey.
Info   : No initialization file found ('/home/rquey/.neperrc').
Info   : ---------------------------------------------------------------
Info   : MODULE  -M loaded with arguments:
Info   : [ini file] (none)
Info   : [com line] n10-id1.tess
Info   : ---------------------------------------------------------------
Info   : Reading input data...
Info   :   - Reading arguments...
Info   : Loading input data...
Info   :   - Loading tessellation...
Info   :     [i] Parsing file 'n10-id1.tess'...
Info   :     [i] Parsed file 'n10-id1.tess'.
Info   : Meshing...
Info   :   - Preparing... (cl = 0.2321) 100%
Info   :   - 0D meshing... 100%
Info   :   - 1D meshing... 100%
Info   :   - 2D meshing... 100% (0.69|0.86/92%| 4%| 4%)
Info   :   - Fixing 2D-mesh pinches...
Info   :   - 3D meshing... 100% (0.89|0.91/100%| 0%| 0%)
Info   : Searching nsets and fasets...
Info   : Writing mesh results...
Info   :   - Preparing mesh...
Info   :   - Mesh properties:
Info   :     > Node number:      295
Info   :     > Elt  number:     1063
Info   :     > Mesh volume:    1.000
Info   :   - Writing mesh...
Info   :     [o] Writing file 'n10-id1.msh'...
Info   :     [o] Wrote file 'n10-id1.msh'.
Info   : Elapsed time: 1.127 secs.
=========================================================================
```

3.1 Arguments

3.1.1 Prerequisites

`-gmsh` *`path_name`* [Prerequisite]
Specify the path of the Gmsh binary (for meshing into triangle and tetrahedral elements).
Possible values: `any`. Default value: `gmsh`.

`-tmp` *`path_name`* [Prerequisite]
Specify the path of the temporary directory (used by Gmsh).
Possible values: `any`. Default value: `"."`.

3.1.2 Input Data

In normal use, the input data is a tessellation file, a raster tessellation file or a mesh file,

`file_name` [Input data]
Specify the name of the input file. It can be a tessellation file (`.tess`), a raster tessellation file (`.tesr`) or a mesh file for remeshing (`.msh`). To load several of them (namely, both a tessellation file and a mesh file for remeshing), combine them with '`,`'. To overwrite the coordinates of the nodes of a mesh, use the syntax '*`file_name`*`:`*`nodecoo_file_name`*', where *`file_name`* is the name of the mesh file and *`nodecoo_file_name`* is the name of the file containing the coordinates of the nodes (see Section B.4 [Position File], page 89). To load only a subregion of a raster tessellation, use the syntax '*`file_name`*`:crop(`*`xmin,xmax,ymin,ymax,zmin,zmax`*`)`', where '*`xmin`*', '*`xmax`*', '*`ymin`*', '*`ymax`*', '*`zmin`*' and '*`zmax`*' are the minimum and maximum positions along x, y and z, respectively. For 2D raster tessellations, the z boundaries can be omitted. To scale the number of points of a raster tessellation, use '*`file_name`*`:scale(`*`factor`*`)`', where *`factor`* is the scaling factor, or '*`file_name`*`:scale(`*`factor_x,factor_y,factor_z`*`)`', where *`factor_x`*, *`factor_y`* and *`factor_z`* are the scaling factor along x, y and z, respectively. For 2D raster tessellations, the z factor can be omitted.
Possible values: `any`. Default value: `none`.

It is also possible to load a mesh to be considered as output mesh (in contrast to loading it as input file). Use option `-o` to avoid overwriting the file. If the file contains meshes of dimensions lower than the tessellation's dimension, these meshes are used and only higher-dimension meshes are generated.

`-loadmesh` *`file_name`* [Input data]
Load a mesh from a file (`.msh` format).
Possible values: `any`. Default value: `none`.

Finally, it is possible to load a set of points. These points are used only for statistics, in option `-statpoint`,

`-loadpoint` *`file_name`* [Input data]
Load points from a file. See Section B.4 [Position File], page 89, for the file format. Provide as argument the file name.
Possible values: `any`. Default value: `none`.

3.1.3 Meshing Options

`-elttype` *`char_string`* [Option]
Specify the type of elements, among '`tri`' for triangular elements, '`quad`' for quadrangular elements, '`quad9`' for 9-node quadrangular elements, '`tet`' for tetrahedral elements and '`hex`' for hexahedral elements. (In 2D, '`tet`' and '`hex`' are treated as '`tri`' and '`quad`', respectively.)
Possible values: `see above`. Default value: `tet in 3D and tri in 2D`.

`-cl or -rcl` *real* [Option]
Specify the absolute or relative characteristic length of the elements. `rcl` is defined relative to the average cell size. The default, `-rcl 1`, leads to a mesh with about 100 elements per cell in average (64 in 2D). For free meshing, it is also possible to define the characteristic length on a per-cell basis, using any mathematical expression based on the variables defined in Section A.2 [Tessellation Keys], page 67, (or Section A.3 [Raster Tessellation Keys], page 70, for a 2D raster tessellation). A typical use is '`-rcl (body>0)?`*`val1`*`:`*`val2`*' to get interior cells meshed with *`rcl=val1`* and boundary cells meshed with *`rcl=val2`*. The second way is to load values from an external file using '`file(`*`file_name`*`)`', where *`file_name`* is the name of the file containing the characteristic length values.
Possible values: `any`. Default value: `-rcl 1`.

`-dim` *char_string* [Option]
Specify the meshing dimension. By default, it is equal to the input data dimension, '`inputdim`'. To get meshes of several dimensions in output, provide the values combined with '`,`'. Provide '`all`' for all and '`none`' for none. Note that the meshes of all dimensions are always written into a `.msh` mesh file unless '`:msh`' is appended to the option argument. If a mesh dimension of 3 is required, but the input data is 2D, the 2D mesh is extruded into a 3D mesh (still made of tetahedra). With '`-format geof`', use '`1,inputdim`' to get the 1D mesh written as lisets.
Possible values: `0 to 3, all, none, inputdim`. Default value: `inputdim`.

`-order` *integer* [Option]
Specify the mesh order. A value of 1 corresponds to 2-node linear elements, 3-node triangular elements, 4-node quadrangular elements, 4-node tetrahedral elements and 8-node hexahedral elements, and a value of 2 corresponds to 3-node linear elements, 6-node triangular elements, 8-node or 9-node quadrangular elements, 10-node tetrahedral elements and 20-node hexahedral elements.
Possible values: `1 or 2`. Default value: `1`.

`-clface or -rclface` *real* [Secondary Option]
Specify the absolute or relative characteristic length of the elements, on a per-face basis. Provide as argument any mathematical expression based on the variables defined in Section A.2 [Tessellation Keys], page 67, or '`default`' (the value inherited from the parent polyhedra). A typical use is '`-rcl (domface==`*`id`*`)?`*`val`*`:default`' to get a finer mesh at domain surface *`id`*. The second way is to load values from an external file using '`file(`*`file_name`*`)`', where *`file_name`* is the name of the file containing the characteristic length values.
Possible values: `any`. Default value: `none`.

`-cledge or -rcledge` *real* [Secondary Option]
Specify the absolute or relative characteristic length of the elements, on a per-edge basis. Provide as argument any mathematical expression based on the variables defined in Section A.2 [Tessellation Keys], page 67, or '`default`' (the value inherited from the parent faces). A typical use is '`-rcl (domedge==`*`id`*`)?`*`val`*`:default`' to get a finer mesh at domain edge *`id`*. The second way is to load values from an external file using '`file(`*`file_name`*`)`', where *`file_name`* is the name of the file containing the characteristic length values.
Possible values: `any`. Default value: `none`.

`-clver or -rclver` *real* [Secondary Option]
Specify the absolute or relative characteristic length of the elements, on a per-vertex basis. Provide as argument any mathematical expression based on the variables defined in Section A.2 [Tessellation Keys], page 67, or '`default`' (the value inherited from the parent edges). A typical use is '`-rcl (domver==`*`id`*`)?`*`val`*`:default`' to get a finer mesh at domain vertex *`id`*. The second way is to load values from an external file using '`file(`*`file_name`*`)`',

where *file_name* is the name of the file containing the characteristic length values.
Possible values: `any`. Default value: `none`.

`-pl` *real* [Secondary option]
Specify the progression factor for the element characteristic lengths. This value is the maximum ratio between the lengths of two adjacent 1D elements.
Possible values: `any >= 1`. Default value: `2`.

`-clratio` *char_string* [Secondary option]
Specify the ratios between the *cl* values along the different coordinate axes. Provide the values combined with '`:`'. For example, '`2:1:1`' leads to elements twice as long in the x direction as in the y and z directions.
Possible values: `none`. Default value: `any`.

`-clmin` *real* [Not recommended option]
Specify the minimum characteristic length of the elements.
Possible values: `any`. Default value: `none`.

The following options define the multimeshing algorithm (for 2D and 3D free meshings). *Multimeshing* consists of using several meshing algorithms concurrently, for each face or polyhedron, until a minimum, target mesh quality is reached. The mesh quality factor, O, accounts for both the element sizes and aspect ratios. It is given by $O = {O_{dis}}^{\alpha} \times {O_{size}}^{1-\alpha}$, where O_{dis} and O_{size} range from 0 (poor quality) to 1 (high quality) and α is a factor equal to 0.8. Therefore, O also ranges from 0 (poor quality) to 1 (high quality).[1] The minimum quality value can be modified using option `-meshqualmin`. The values of O and O_{dis} can be modified using options `-meshqualexpr` and `-meshqualdisexpr`. The value of the target mesh quality significantly influences meshing speed and output mesh quality. A value of 0 provides the fastest meshing while a value of 1 provides the best-quality meshing. The default value provides an effective balance. 2D and 3D meshings are achieved using the Gmsh[2] and Netgen[3] libraries (options `-mesh2dalgo` and `-mesh3dalgo`).

`-meshqualmin` *real* [Option]
Specify the minimum, target value of mesh quality, O, as defined by option `-meshqualexpr`.
Possible values: `0 to 1`. Default value: `0.9`.

`-meshqualexpr` *char_string* [Option]
Specify the expression of mesh quality, O, as a function of *Odis* and *Osize*.
Possible values: `any`. Default value: `Odis^0.8*Osize^0.2`.

`-meshqualdisexpr` *char_string* [Secondary option]
Specify the expression of the mesh element distortion parameter, *Odis*, as a function of the element distortion parameter *dis*.
Possible values: `any`. Default value: `dis^(exp((dis^0.1)/(dis^0.1-1)))`.

`-mesh2dalgo` *char_string* [Secondary option]
Specify the 2D meshing algorithms, combined with '`,`'. The available values are `mead` (MeshAdapt), `dela` (Delaunay) and `fron` (Frontal).
Possible values: `mead, dela, fron`. Default value: `mead,dela,fron`.

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[1] See *R. Quey, P.R. Dawson and F. Barbe, Large-scale 3D random polycrystals for the finite element method: Generation, meshing and remeshing, Comput. Methods Appl. Mech. Engrg., vol. 200, pp. 1729-1745, 2011.*

[2] *Ch. Geuzaine and J.-F. Remacle, Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities, International Journal for Numerical Methods in Engineering, 79, 1309–1331, 2009.*

[3] *J. Schoberl, Netgen, an advancing front 2d/3d-mesh generator based on abstract rules. Comput. Visual. Sci., 52, 1–41, 1997.*

`-mesh3dalgo` *char_string* [Secondary option]
Specify the 3D meshing algorithms, combined with '`,`'. Each algorithm has format '*mesh*`:`*opti*', where *mesh* and *opti* stand for the meshing and mesh optimization algorithms. The available values of *mesh* are currently limited to `netg` (Netgen). The available values of *opti* are '`gmsh`' (Gmsh), '`netg`' (Netgen), '`gmne`' (Gmsh + Netgen) and '`none`' for none.
Possible values: `netg:none, netg:gmsh, netg:netg, netg:gmne`. Default value: `netg:gmsh,netg:netg,netg:gmne`.

`-interface` *char_string* [Secondary option]
Specify the type of interface meshing. Provide '`continuous`' for a continuous mesh at interfaces, with shared nodes between neighbor element sets (which are associated to the tessellation cells). Provide '`discontinuous`' for a discontinuous mesh at interfaces, with distinct nodes for the neighbor element sets. Provide '`cohesive`' for cohesive elements at interfaces, joining the neigbour element sets. In the case of a multiscale tessellation, it is possible to provide a different value for each scale using the '`::`' separator (if fewer values than tessellation scales are provided, the last provided value is used for all higher scales). See option `-faset` for the output format.
Possible values: `see above`. Default value: `continuous`.

`-mesh2dpinchfix` *logical* [Secondary option]
Apply 2D-mesh pinches correction after 2D meshing. Disable only if you really know what you are doing.
Possible values: `0 or 1`. Default value: `1`.

3.1.4 Raster Tessellation Meshing Options

Raster tessellation meshing implies interface reconstruction, interface mesh smoothing then remeshing. The following options enable the control of interface smoothing.

`-tesrsmooth` *char_string* [Secondary option]
Method for smoothing the interface meshes reconstructed from raster tessellations. Laplacian smoothing ('`laplacian`') is an iterative method that modifies the coordinates of a node using the coordinates of the neighboring nodes. At iteration i, the position of a node, X_i, is calculated from its previous position, X_{i-1}, and the position of the barycentre of the neighboring nodes (weighted barycentre, considering the inverse of the distance between the node and the neighbor), X^n_{i-1}, as follows: $X_i = (1-A)\,X_{i-1} + A\,X^n_{i-1}$. $A \in [0, 1]$ is an adjustable parameter (see option `-tesrsmoothfact`). The number of iterations is set by option `-tesrsmoothitermax`. There is no stop criterion, so `itermax` will always be reached.
Possible values: `laplacian or none`. Default value: `laplacian`.

`-tesrsmoothfact` *real* [Secondary option]
Specify the factor used for the interface mesh smoothing (A in option `-tesrsmooth`).
Possible values: `0 to 1`. Default value: `0.5`.

`-tesrsmoothitermax` *integer* [Secondary option]
Specify the number of iterations used for interface mesh smoothing.
Possible values: `any >= 0`. Default value: `5`.

3.1.5 Mesh Cleaning Options

The following options are specific to mapped meshing of raster tessellations containing voids.

`-clean` *integer* [Secondary option]
Clean the mesh so that it consists of a set of connected elements. Provide as argument the level of cleaning. A value of `1` indicates that two elements should be considered connected to each other if they share at least a vertex. A value of `2` indicates that two elements should

be considered connected to each other if they share at least a face. Using this option, the elements (or bunches of elements) that are not connected to the main skeleton are removed. Possible values: `0 to 2`. Default value: `0`.

`-singnodedup` *logical* [Secondary option]
Duplicate nodes which are the subject of singularity. Such a node belongs to several elements which share only a node or an edge, which provides a singular behavior: in Mechanics, it corresponds to imposing a common displacement, while the point can carry no stress, and in Thermics, it corresponds to imposing a given temperature at a particular location shared by two bodies, while the location can carry no heat flux. When this option is enabled, such a node is duplicated, so that each body has its own node. Option `-dupnodemerge` allows one to merge back duplicate nodes.
Possible values: `0 or 1`. Default value: `0`.

`-dupnodemerge` *real* [Secondary option]
Merge duplicate nodes. Provide as argument the distance between nodes below which two nodes are merged. Note that Neper does not generate meshes with duplicate nodes, except using options `-singnodedup` or `-interface`.
Possible values: `0`. Default value: `any>0`.

3.1.6 Transformation Options

`-transform` *char_string(...)* [Option]
Apply transformations to a mesh. The following transformations can be applied:
• '`scale(`*x_fact*`,`*y_fact*`,`*z_fact*`)`' scales a mesh by *x_fact*, *y_fact* and *z_fact* along directions *x*, *y* and *z*, respectively. For a 2D mesh, *z_fact* can be omitted.
• '`rotate(`*axis_x*`,`*axis_y*`,`*axis_z*`,`*angle*`)`' rotates a mesh about the centre and by an axis/angle pair.
• '`translate(`*dist_x*`,`*dist_y*`,`*dist_z*`)`' translates a mesh by distances *dist_x*, *dist_y* and *dist_z* along directions *x*, *y* and *z*, respectively.
• '`mooth(`*fact*`,`*itermax*`,`*type*`)`' smooths the interfaces of a mesh by Laplacian smoothing (use only if you know what you are doing). Laplacian smoothing is an iterative method that modifies the coordinates of a node using the coordinates of the neighboring nodes. At iteration *i*, the position of a node, X_i, is calculated from its previous position, X_{i-1}, and the position of the barycentre of the neighboring nodes (weighted barycentre, considering the inverse of the distance between the node and the neighbor), X^n_{i-1}, as follows: $X_i = (1 - fact)\, X_{i-1} + fact\, X^n_{i-1}$; $0 \leq fact \leq 1$. *itermax* iterations are applied. *type* defines the nodes used for smoothing and can be '`all`' for all nodes or '`interior`' for interior nodes.
• '`explode(`*fact*`)`' to produce a roughly "exploded" mesh, for which elsets are apart from each other (or cohesive elements become thick). To be used in conjunction with `-interface discontinuous or cohesive`. '*fact*' is a factor controlling the distance between elsets.
• '`slice(d,a,b,c)`' slices a 3D mesh by the (oriented) plane of equation $a\,x + b\,y + c\,z = d$ (yielding to a 2D mesh).
Possible values: `see above`. Default value: `none`.

3.1.7 Mesh Partitioning Options

Mesh partitioning is achieved using the libScotch library[4]. The principle of mesh partitioning is to create partitions of the same size while minimizing the interfaces between them. This attempts to distribute an equal load to all computation units and minimizes communications between them, and therefore minimizes the total computation time. There are two available strategies

[4] *F. Pellegrini, Scotch and libScotch 5.1 User's Guide, INRIA Bordeaux Sud-Ouest, ENSEIRB & LaBRI, UMR CNRS 5800, 2008.*

for mesh partitioning. The first one creates partitions and arranges them independently of each other, while the second one consists of optimizing the size and arrangment of the partitions based on a given computer cluster architecture to minimize computation time further. For those clusters that are made of nodes containing several cores each, the communication time between cores on a common node is much lower than the communication time between cores of different nodes. To minimize the global communication time, partitions which are processed by cores of the same node can be grouped together (on modern architectures, the gain remains marginal). Partitioning is applied to the higher-dimension mesh and renumbers nodes and elements by ascending partition number. This can be managed using options beginning with `-part`.

`-part` *integer or char_string* [Option]
Specify the number of partitions or a computer cluster architecture. Using the first option, the number of partition can be any. At the opposite, for a computer cluster architecture, the total number of partitions must be a power of 2. An architecture can be specified in two ways. First, for clusters that contain nodes made of several cores, the number of nodes and the number of cores per node can be combined using the '`:`' separator. A ratio of 10 is considered between the computation time between cores located on different nodes and the one between cores of the same node. Second, the name of a file describing the cluster architecture in the Scotch format can be provided.
Possible values: `any`. Default value: `none`.

`-partbalancing` *real* [Secondary option]
Specify the rate of element partition balancing (the nominal partitioning applies to the nodes, while the element partitions are determined afterwards and can be somewhat unbalanced). This option allows for the enforcement of equal balancing, but getting equal balance is highly CPU-intensive.
Possible values: `0 to 1`. Default value: `0.5`.

`-partmethod` *char_string* [Secondary option]
Specify the partitioning method. Provide the partitioning expression in Scotch's jargon, or '`none`' for none.
Possible values: `any`. Default value: `see the source`.

3.1.8 Field Transport Options

`-transport` *char_string:char_string:file_name,...* [Option]
Transport data from a parent mesh to a child mesh. The parent mesh is the input mesh and the child mesh is the result mesh (created by remeshing or loaded with `-loadmesh`). A transport entry must have format '*entity_type*`:`*data_type*`:`*file_name*', where '*entity_type*' must be '`node`' or '`elt`', '*data_type*' is the type of data, under format '`integer`*X*' or '`real`*X*', where *X* is the dimension, and *file_name* is the name of the file containing the parent data. For several data transports, combine the transport entries with '`,`'. Nodal data are transported by interpolation using the shape functions (2D only). Elemental data are transported as specified by `-transporteltmethod`.
Possible values: `any`. Default value: `none`.

`-transporteltmethod` *char_string:char_string...* [Secondary option]
Specify the method to transport elemental data from the parent mesh to the child mesh. For each element of the child mesh, its centre, c, is considered. Use '`distance`' to choose, for each element of the child mesh (of centre c), the element of the parent mesh whose centre is the closest to c, or '`location`' to choose the element c belongs to.
Possible values: `see above`. Default value: `distance`.

3.1.9 Output Options

`-o` *`file_name`* [Option]
Specify the output file name.
Possible values: `any`. Default value: `input basename`.

`-format` *`char_string`* [Option]
Specify the format of the output file(s). Mesh formats are: the native (Gmsh-style) '`msh`', the Gmsh version 4 '`msh4`', the VTK '`vtk`', the Abaqus '`inp`' and the Z-set '`geof`'. For '`msh`', append '`:`*`format`*' to specify the format, which can be '`ascii`' or '`binary`' (default '`ascii`'). To get the orientation section of the '`msh`' file (optional FEPX input), provide '`ori`'. To get a boundary conditions file (optional FEPX input), provide '`bcs`'. To get a periodicity file, provide '`per`'. To get a tessellation file (reconstructed from the mesh) , provide '`tess`'. Combine arguments with '`,`'.
Possible values: `see above`. Default value: `msh`.

`-nset` *`char_string`* [Option]
Specify the node sets to provide, among: `faces`, `edges`, `vertices` for all domain faces, edges and vertices, and `facebodies` and `edgebodies` for all face and edge bodies (interiors). Provide `all` for all and `none` for none. To get the node sets corresponding to individual entities, provide their labels. For a cuboidal domain, they are `[x-z][0,1]` for the domain faces, `[x-z][0,1][x-z][0,1]` for the edges, and `[x-z][0,1][x-z][0,1][x-z][0,1]` for the vertices. For a cylindrical domain, they are `z[0,1]` for the z faces, and `f[1,2,...]` for the faces on the circular part of the domain. For other domains, they are `f[1,2,...]` for the faces. For cylindrical and other types of domains, the edge and vertex labels are obtained from the face labels as for cuboidal domains. For a 2D mesh (generated from a 2D tessellation), the labels are `[x-y][0,1]` for the edges and `[x-y][0,1][x-y][0,1]` for the vertices. Append '`body`' to a label to get only the body (interior) nodes of the set. Combine labels with '`,`'.
Possible values: `see above`. Default value: `faces in 3D and edges in 2D`.

`-faset` *`char_string`* [Option]
Specify the element surface meshes (edge meshes in 2D) to output. Use '`faces`' for all domain faces. To get the meshes of individual faces, provide their labels (see option `-nset`). For internal mesh faces (edges in 2D) as created by '`-interface discontinuous`', provide '`internal`'. Combine them with '`,`'. Provide `none` for none.
Possible values: `see above`. Default value: `all`.

`-elset` *`char_string`* [Secondary option]
Specify the element sets to output. The argument can be: `default` for the default element sets (those corresponding to the input tessellation cells), or an expression of the form '*`elset_label`*`:`*`elset_definition`*', where *`elset_label`* is a custom elset label and *`elset_definition`* is an expression defining the elements belonging to the elset, defined from the variables provided in Section A.6 [Mesh Keys], page 73. Combine arguments with '`,`'.
Possible values: `see above`. Default value: `default`.

`-performat` *`char_string`* [Option]
Specify the format of the `.per` output file. The available formats are: the native `msh`, the plain `plain` and the Z-set `geof`.
Possible values: `see above`. Default value: `msh`.

3.1.10 Post-Processing Options

The following options provide general statistics on the (highest-dimension) mesh ('`mesh`'), 0D mesh ('`mesh0d`'), 1D mesh ('`mesh1d`'), 2D mesh ('`mesh2d`'), 3D mesh ('`mesh3d`') and cohesive-element mesh ('`meshco`').

`-statmesh` *char_string* [Post-processing]
Provide statistics on the highest-dimension mesh. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stmesh`.

`-statmesh0d` *char_string* [Post-processing]
Provide statistics on the 0D mesh. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stmesh0d`.

`-statmesh1d` *char_string* [Post-processing]
Provide statistics on the 1D mesh. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stmesh1d`.

`-statmesh2d` *char_string* [Post-processing]
Provide statistics on the 2D mesh. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stmesh2d`.

`-statmesh3d` *char_string* [Post-processing]
Provide statistics on the 3D mesh. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stmesh3d`.

`-statmeshco` *char_string* [Post-processing]
Provide statistics on the cohesive-element mesh. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stmeshco`.

The following options provide statistics on the nodes ('`nodes`'), (highest-dimension) elements ('`elt`') and element sets ('`elset`'), 0D elements ('`elt0d`') and element sets ('`elset0d`'), 1D elements ('`elt1d`') and element sets ('`elset1d`'), 2D elements ('`elt2d`') and element sets ('`elset2d`'), 3D elements ('`elt3d`') and element sets ('`elset3d`'), and cohesive elements ('`eltco`') and element sets ('`elsetco`').

`-statnode` *char_string* [Post-processing]
Provide statistics on the nodes. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stnode`.

`-statelt` *char_string* [Post-processing]
Provide statistics on the highest-dimension elements. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stelt`.

`-statelt0d` *char_string* [Post-processing]
Provide statistics on the 0D elements. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with ‘,’.
Possible values: `any`. Default value: `none`.
Result file: extension `.statelt0d`.

`-statelt1d` *char_string* [Post-processing]
Provide statistics on the 1D elements. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with ‘,’.
Possible values: `any`. Default value: `none`.
Result file: extension `.statelt1d`.

`-statelt2d` *char_string* [Post-processing]
Provide statistics on the 2D elements. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with ‘,’.
Possible values: `any`. Default value: `none`.
Result file: extension `.statelt2d`.

`-statelt3d` *char_string* [Post-processing]
Provide statistics on the 3D elements. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with ‘,’.
Possible values: `any`. Default value: `none`.
Result file: extension `.statelt3d`.

`-statelset` *char_string* [Post-processing]
Provide statistics on the highest-dimension element sets. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with ‘,’.
Possible values: `any`. Default value: `none`.
Result file: extension `.statelset`.

`-statelset0d` *char_string* [Post-processing]
Provide statistics on the 0D element sets. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with ‘,’.
Possible values: `any`. Default value: `none`.
Result file: extension `.statelset0d`.

`-statelset1d` *char_string* [Post-processing]
Provide statistics on the 1D element sets. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with ‘,’.
Possible values: `any`. Default value: `none`.
Result file: extension `.statelset1d`.

`-statelset2d` *char_string* [Post-processing]
Provide statistics on the 2D element sets. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with ‘,’.
Possible values: `any`. Default value: `none`.
Result file: extension `.statelset2d`.

`-statelset3d` *char_string* [Post-processing]
Provide statistics on the 3D element sets. Provide as argument the keys as described in Section A.6 [Mesh Keys], page 73, combined with ‘,’.
Possible values: `any`. Default value: `none`.
Result file: extension `.statelset3d`.

`-statpoint` *char_string* [Post-processing]
Provide statistics on points. The points must be loaded with option `-loadpoint`. Provide as argument the keys as described in Section A.7 [Point Keys], page 74, combined with '`,`'.
Possible values: `any`. Default value: `none`.
Result file: extension `.stpoint`.

3.1.11 Advanced Options

These advanced options set running conditions for the meshing libraries (2D and 3D meshing),

`-mesh3dclreps` *real* [Secondary option]
Specify the relative tolerance on the average element characteristic length of each polyhedron (compared to `cl`). The value can also be defined on a per-cell basis, using any mathematical expression based on the variables defined in Section A.2 [Tessellation Keys], page 67, or by loading values from an external file, using '`file(`*file_name*`)`', where *file_name* is the name of the file containing the values. As Neper proceeds iteratively to adjust the average element characteristic length, this is a highly CPU-intensive capability, and low values will increase computation time significantly.
Possible values: `any`. Default value: `0.02`.

`-mesh2dmaxtime` *real* [Secondary option]
Specify the maximum processing time allowed to the meshing library for meshing a tessellation face (in seconds).
Possible values: `any`. Default value: `1000`.

`-mesh2drmaxtime` *real* [Secondary option]
Specify a factor used to determine the maximum processing time allowed to the meshing library for meshing a tessellation face. This option is similar to `-mesh2dmaxtime`, but the actual maximum time is the product of the maximum processing time of the previous meshings by the value provided in argument.
Possible values: `any`. Default value: `100`.

`-mesh2diter` *integer* [Secondary option]
Specify the maximum number of 2D meshing attempts for a particular face (in the rare case of failure).
Possible values: `any`. Default value: `3`.

`-mesh3dmaxtime` *real* [Secondary option]
Specify the maximum processing time allowed to the meshing library for meshing a tessellation polyhedron (in seconds).
Possible values: `any`. Default value: `1000`.

`-mesh3drmaxtime` *real* [Secondary option]
Specify a factor used to determine the maximum processing time allowed to the meshing library for meshing a tessellation polyhedron. This option is similar to `-mesh3dmaxtime`, but the actual maximum time is the product of the maximum processing time of the previous meshings by the value provided in argument.
Possible values: `any`. Default value: `100`.

`-mesh3diter` *integer* [Secondary option]
Specify the maximum number of 3D meshing attempts for a particular polyhedron (in the rare case of failure).
Possible values: `any`. Default value: `3`.

3.2 Output Files

3.2.1 Mesh

The mesh can be written in the following formats,

- native format: file `.msh`. See Section B.5 [Mesh File (`.msh`)], page 89, for the file syntax.
- native format / orientations (optional FEPX file): file `.ori`. It contains the '`$ElsetOrientations`' and '`$ElementOrientations`' sections of the msh file.
- native format / periodicity: file `.per`.
- native format / boundary conditions (optional FEPX file): file `.bcs`.
- Gmsh format version 4: file `.msh4`
- VTK format: file `.vtk`
- Abaqus format: file `.inp`
- Z-set format: file `.geof`

3.2.2 Interfaces

- File `.intl`. For each 2D interface, the file provide (one 2D interface per line): the labels of the two element sets of the interface.

3.2.3 Statistics

Statistics files are provided for nodes, elements, element sets and points. They are formatted with one entity per line. Each line contains the data specified to the corresponding `-stat` option and described in Section A.6 [Mesh Keys], page 73.

- Node statistics file, `.stnode`.
- (Highest-dimension) mesh statistics file, `.stmesh`.
- (Highest-dimension) element statistics file, `.stelt`.
- (Highest-dimension) element set statistics file, `.stelset`.
- 0D mesh statistics file, `.stmesh0d`.
- 1D mesh statistics file, `.stmesh1d`.
- 2D mesh statistics file, `.stmesh2d`.
- 3D mesh statistics file, `.stmesh3d`.
- Cohesive-element mesh statistics file, `.stmeshco`.
- 0D element statistics file, `.stelt0d`.
- 1D element statistics file, `.stelt1d`.
- 2D element statistics file, `.stelt2d`.
- 3D element statistics file, `.stelt3d`.
- 0D element set statistics file, `.stelset0d`.
- 1D element set statistics file, `.stelset1d`.
- 2D element set statistics file, `.stelset2d`.
- 3D element set statistics file, `.stelset3d`.
- Point statistics file, `.stpoint`.

3.3 Examples

Below are some examples of use of neper -M.

1. Mesh tessellation `n100-id1.tess`.
   ```
   $ neper -M n100-id1.tess
   ```
2. Mesh 2D raster tessellation `n100-id1.tesr`.
   ```
   $ neper -M n100-id1.tesr
   ```
3. Mesh tessellation `n100-id1.tess` with a mesh size of rcl = 0.5 and in 2nd-order elements.
   ```
   $ neper -M n100-id1.tess -rcl 0.5 -order 2
   ```
4. Mesh tessellation `n100-id1.tess` with small elements for the interior cells and bigger elements for the boundary cells.
   ```
   $ neper -M n100-id1.tess -rcl "body!=0?0.2:0.5"
   ```
5. Remesh mesh `n150_def.msh` (comprising poor-quality elements) into a clean, new mesh. Transport the scalar data of file `n150_def.data` from the deformed mesh to the new mesh.
   ```
   $ neper -M n150.tess,n150_def.msh -transport elt:real1:n150_def.data
     -rcl 0.5 -o n150_new
   ```
6. Mesh tessellation `n100-id1.tess` and divide the mesh into 8 partitions.
   ```
   $ neper -M n100-id1.tess -part 8
   ```
7. Mesh tessellation `n100-id1.tess` into regular hexahedral elements (non-conformal mesh).
   ```
   $ neper -M n100-id1.tess -elt hex
   ```
8. Mesh tessellation `n100-id1.tess` and get, for each element, its radius ratio and its volume.
   ```
   $ neper -M n100-id1.tess -statelt rr,vol
   ```
9. Mesh tessellation `n100-id1.tess` and get the number of nodes and elements of the mesh.
   ```
   $ neper -M n100-id1.tess -statmesh nodenb,eltnb
   ```

4 Simulation Module (-S)

Module -S is the module for post-processing simulation results. Its primarily aims at reformatting an FEPX raw result directory into a *simulation directory* (see Section B.6 [Simulation Directory (`.sim`)], page 92), which is as simple as running '`neper -S fepx_res_dir`', where '*`fepx_res_dir`*' is the FEPX raw result directory. All FEPX raw results are reformatted by default, but a list of specific results (or new results) can be specified using options `-noderes` and `-eltres`. The simulation directory has a simple structure and can be loaded in module -V for result visualization.

Here is what a typical run of module -S looks like:

```
$ neper -S fepx-simulation

=======================    N   e   p   e   r    ======================
Info   : A software package for polycrystal generation and meshing.
Info   : Version 4.0.0
Info   : Built with: gsl|muparser|opengjk|openmp|nlopt|libscotch (full)
Info   : Running on 8 threads.
Info   : <http://neper.info>
Info   : Copyright (C) 2003-2020, and GNU GPL'd, by Romain Quey.
Info   : Loading initialization file '/home/rquey/.neperrc'...
Info   : ---------------------------------------------------------------
Info   : MODULE  -S loaded with arguments:
Info   : [ini file] (none)
Info   : [com line] fepx-simulation
Info   : ---------------------------------------------------------------
Info   : Reading input data...
Info   :   - Reading arguments...
Info   : Writing simulation directory from FEPX result directory...
Info   :     [o] Writing directory 'fepx-simulation.sim'...
Info   :   - Parsing FEPX results...
Info   :     [i] Parsing file 'fepx-simulation/post.report'...
Info   :     [i] Parsed file 'fepx-simulation/post.report'.
Info   :     > Partition number: 8.
Info   :     > Step      number: 10.
Info   :     > Node      number: 2752.
Info   :     > Element   number: 1596.
Info   :   - Writing report file...
Info   :     [o] Writing file 'fepx-simulation.sim/report'...
Info   :     [o] Wrote file 'fepx-simulation.sim/report'.
Info   :   - Writing inputs...
Info   :     [o] Writing directory 'fepx-simulation.sim/inputs'...
Info   :       . simulation.tess...
Info   :       . simulation.msh...
Info   :       . simulation.config...
Info   :     [o] Wrote directory 'fepx-simulation.sim/inputs'.
Info   :   - Writing results...
Info   :     [o] Writing directory 'fepx-simulation.sim/results'...
Info   :       . coo...       100%
Info   :       . ori...       100%
Info   :     [o] Wrote directory 'fepx-simulation.sim/results'.
```

```
Info   :     [o] Wrote directory 'fepx-simulation.sim'.
Info   : Elapsed time: 0.075 secs.
================================================================================
```

4.1 Arguments

4.1.1 Input Data

directory_name [Input data]
Specify the name of the input directory. It can be an FEPX raw result directory or a simulation directory.
Possible values: `any`. Default value: `none`.

4.1.2 Results Options

Below are options to define the results to write. In the case where a simulation directory is loaded as input, the specified results add to the existing results.

`-noderes` *char_string* [Option]
Specify the nodal results to output. Provide '`none`' for none, '`inputres`' for all FEPX raw results, '*`res`*' for a specific FEPX raw results, or any expression based on the variables listed in Section A.6 [Mesh Keys], page 73. To provide several values, combine them with '`,`'.
Possible values: `any`. Default value: `inputres`.

`-eltres` *char_string* [Option]
Specify the elemental results to output. Provide '`none`' for none, '`inputres`' for all FEPX raw results, '*`res`*' for a specific FEPX raw results, or any expression based on the variables listed in Section A.6 [Mesh Keys], page 73. To provide several values, combine them with '`,`'.
Possible values: `any`. Default value: `inputres`.

4.1.3 Output Options

`-o` *directory_name* [Option]
Specify the name of the output simulation directory (the default `.sim` extension is not added to the argument).
Possible values: `any`. Default value: *`fepx_result_directory`*`.sim`.

4.2 Output Directory

The output directory is

- Simulation directory `.sim`

  It contains the input files and the results of the simulation. See Section B.6 [Simulation Directory (`.sim`)], page 92, for details on its content.

4.3 Examples

Below are some examples of use of neper -S.

1. Transform an FEPX raw result directory into a simulation directory of specified name.

   ```
   $ neper -S fepx-simulation -o foo
   ```

2. Transform an FEPX raw result directory into a simulation directory of specified results: the nodal '`coo`' and the elemental '`ori`'.

   ```
   $ neper -S fepx-simulation -noderes coo -eltres ori
   ```

5 Visualization Module (-V)

Module -V is the module for visualizing tessellations, meshes and simulation results as publication-quality PNG images[1] or as VTK files, for interactive visualization. Results can be defined from internal data, data loaded from external files or a simulation directory as generated by module -S. For the PNG images, it is possible to set different attributes of the tessellations and meshes such as the node coordinates, or the colors and transparencies of the different entities. Point data can also be represented, using symbols of specified sizes and colors. Slice views can also be generated.

Contrary to other modules, module -V processes the command arguments one after the other. Typically, using module -V consists of loading a tessellation or a mesh, then data fields to render them — which is done all at once by loading a simulation directory as generated by module -S. The data can apply to the tessellation entities: polyhedra, faces, edges and vertices, to the mesh entities: 3D, 2D, 1D and 0D elements and nodes, and to points (options beginning with `-data`). In the case of a PNG output file, many aspects of the scene can be set into fine detail: the entities that are to be visible, for example particular tessellation cells, element sets or elements, can be specified (options beginning with `-show`); the way they are plotted (camera position and angle, projection type, image size, etc.) can also be set up (options beginning with `-camera` or `-image`), and the coordinate system can be added.

Here is what a typical run of module -V looks like:

```
$ neper -V n10-id1.tess,n10-id1.msh -dataelsetcol id -print img

========================    N   e   p   e   r    ======================
Info   : A software package for polycrystal generation and meshing.
Info   : Version 4.0.0
Info   : Built with: gsl|muparser|opengjk|openmp|nlopt|libscotch (full)
Info   : Running on 8 threads.
Info   : <http://neper.info>
Info   : Copyright (C) 2003-2020, and GNU GPL'd, by Romain Quey.
Info   : No initialization file found ('/home/rquey/.neperrc').
Info   : ---------------------------------------------------------------
Info   : MODULE  -V loaded with arguments:
Info   : [ini file] (none)
Info   : [com line] n10-id1.tess,n10-id1.msh -dataelsetcol id -print img
Info   : ---------------------------------------------------------------
Info   : Loading tessellation...
Info   :     [i] Parsing file 'n10-id1.tess'...
Info   :     [i] Parsed file 'n10-id1.tess'.
Info   : Loading mesh...
Info   :     [i] Parsing file 'n10-id1.msh'...
Info   :     [i] Parsed file 'n10-id1.msh'.
Info   : Reconstructing mesh...
Info   : Reading data (elset3d, col)...
Info   : Printing image...
Info   :     [o] Writing file 'img.pov'...
Info   :   - Printing mesh...
Info   :     > Reducing data...
Info   :       . 3D...
```

[1] The POV-Ray ray-tracing library is used for generating the images.

```
Info   :       . 2D...
Info   :       . Number of 3D elt faces reduced by  90% (to 418).
Info   :       . Number of 3D elt edges reduced by  50% (to 627).
Info   :       . Number of 0D elts      reduced by 100% (to 0).
Info   :     [o] Wrote file 'img.pov'.
Info   :   - Generating png file (1200x900 pixels)...
Info   :     [o] Writing file 'img.png'...
Info   :     [o] Wrote file 'img.png'.
Info   : Printing scale...
Info   : Elapsed time: 1.546 secs.
==========================================================================
```

5.1 Arguments

5.1.1 Prerequisites

`-povray` *path_name* [Prerequisite]
Specify the path of the POV-Ray binary (for generating PNG images).
Possible values: `any`. Default value: `povray`.

5.1.2 Input Data

file_name [Input data]
Specify the names of the input file(s) or directory. The files can be a tessellation file (`.tess`), a raster tessellation file (`.tesr`), a mesh file (`.msh`) or a point file (see Section B.4 [Position File], page 89). The directory must be a simulation directory as generated by module -S. To load several of them, combine them with '`,`'.
Possible values: `any`. Default value: `none`.

When a simulation directory is loaded as input, it is possible to set the simulation step to consider using the following option,

`-simstep` *integer* [Option]
Specify the simulation step (`0` for the initial state).
Possible values: `any`. Default value: `0`.

The data internal to the simulation directory have the same status as internal data (such as, for instance, the nominal element orientations stored in the mesh file) and can therefore be loaded (with options `-data*`) more simply than with standard external files. For example, coloring elements from orientations can be done using, instead of the standard '`-dataeltcol "ori:file(`*simulation_directory*`/res/ori/ori.step2)"`' or, when '`-simstep 2`' was invoked before, '`-dataeltcol ori`' (since the variable is self-defined and the simulation step is known, Neper will figure out which file to use).

5.1.3 Space Options

The following option enables the definition of the space which the input data (tessellation, mesh, point, etc.) are defined in. The space is most generally real (physical) space, but can be defined as Rodrigues orientation space, which makes it possible to account for its distortion.[2]

`-space` *char_string* [Secondary option]
Specify the space which the input data are defined in. Use '`real`' for real space or '`rodrigues`' for Rodrigues orientation space.
Possible values: `see above`. Default value: `real`.

[2] It currently only affects the arguments of `-datapointrad`.

5.1.4 Tessellation Data Loading and Rendering

The following options enable the definition of the properties (color and size) of the tessellation cells or entities (polyhedra, faces, edges and vertices). This can be done either directly, by specifying the property values (e.g. the RGB channel values for color) or indirectly, e.g. using scalar values that are converted in color using a given *color scheme*. In this case, a scale image is generated in addition to the tessellation image. The scale properties can be set up (minimum, maximum and tick values).

The following options apply to the cells of a tessellation or a raster tessellation, independently of its dimension,

`-datacellcol` *`char_string`* [Option]

Set the colors of the tessellation cells, which can be done in two main different ways.

(i) Colors can be specified directly as follows:

• '*`value`*', where '*`value`*' can be a color that applies to all cells, or '`file(`*`file_name`*`)`' for a file containing the individual colors (see Section A.11 [Colors and Color Maps], page 76).

(ii) Colors can be set from data using an argument of the general form '*`data_type`*`:`*`data_value`*', which can be shortened[3] to '*`data_value`*' in the frequent case where the data type can be unambiguously determined from the data value:

• '`int:`*`data_value`*' for integer values represented using a color palette, where '*`data_value`*' can be an integer-value expression such as '`id`' or '`mode`' and (see Section A.2 [Tessellation Keys], page 67), or '`file(`*`file_name`*`)`' for a file containing the individual values.

• '`real:`*`data_value`*' for real values represented using a smooth color scale, where '*`data_value`*' can be a real-value expression such as '`x`' or '`vol`' (see Section A.2 [Tessellation Keys], page 67), or '`file(`*`file_name`*`)`' for a file containing the individual values.

• '`ori:`*`data_value`*' for the crystal orientations (when applicable), where '*`data_value`*' can be an orientation (see Section A.9 [Rotations and Orientations], page 75), '`internal`' to use the internal orientations, or '`file(`*`file_name`*`,[des=`*`descriptor`*`])`' for a file containing the individual values (see Section A.9 [Rotations and Orientations], page 75). Because '`ori`' is self-defined, '*`data_value`*' can also be omitted in the case where internal orientations are to be used.

The color schemes used to determine the colors from the data can be fine-tuned using options `-data*colscheme`.

Possible values: `any`. Default value: `white`.

`-datacellcolscheme` *`char_string`* [Option]

Set the color scheme used to get colors from the data of the tessellation cells loaded with option `-datacellcol`. The type of color scheme depends on the type of data.

• For integer values, the color scheme is '`palette`' (see Section A.11 [Colors and Color Maps], page 76).

• For real values, several color schemes are available (see Section A.11 [Colors and Color Maps], page 76) and the default is '`viridis`'.

• For crystal orientations (cubic symmetry is assumed), the color scheme can be: '`ipf(`*`dir`*`)`' for IPF coloring using direction '*`dir`*', where '*`dir`*' should be one of '`x`', '`y`' or '`z`' (default '`z`'), '`rodrigues`' for Rodrigues vector coloring (default is inside the fundamental region, can be bounded using '`rodrigues(`*`max`*`)`', where *max* is the half-length along a direction), '`axis`' for rotation axis coloring, '`angle`' for rotation angle coloring (can be bounded using '`angle(`*`max`*`)`', where *max* is the maximum angle (in radian)) and '`axis-angle`' for rotation axis / angle coloring (can be bounded using '`axis-angle(`*`max`*`)`', where *max* is the maximum angle (in radian)).

Possible values: `see above`. Default value: `"palette" for integer values, "viridis" for real values and "rodrigues" for crystal orientations`.

[3] This ensures backward compatibility with versions 3.x.

`-datacelltrs` *real* [Option]
Set the transparency of the tessellation cells. Provide as argument a value that applies to all cells or '`file(`*file_name*`)`' to load values from a file.
Possible values: `0 to 1`. Default value: `0`.

`-datacellscale` *char_string* [Option]
Set the scale relative to the '`-datacellcol real`' data. Provide as argument the start and end values, combined with '`:`'. To specify the intermediate values, provide as argument the start value, the intermediate values and the end value, combined with '`:`'. The labels of the scale follow the format used for the start value.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-datacellscaletitle` *char_string* [Option]
Set the title of the scale relative to the '`-datacellcol real`' data.
Possible values: `any`. Default value: `none`.

For tessellations, it is also possible to set data on a per-entity basis,

`-datapolycol` *char_string* [Option]
Set the colors of the tessellation polys. See option `-datacellcol` for the argument format.
Possible values: `any`. Default value: `white`.

`-datapolycolscheme` *char_string* [Option]
Set the color scheme used to get colors from the data of the tessellation faces loaded with option `-datapolycol`. See option `-datacellcolscheme` for the argument format.
Possible values: `see option -datacellcolscheme`. Default value: `see option -datacellcolscheme`.

`-datapolytrs` *real* [Option]
Set the transparency of the tessellation polyhedra. Provide as argument a value that applies to all polyhedra or '`file(`*file_name*`)`' to load values from a file.
Possible values: `0 to 1`. Default value: `0`.

`-datapolyscale` *char_string* [Option]
Set the scale relative to the '`-datapolycol real`' data. Provide as argument the start and end values, combined with '`:`'. To specify the intermediate values, provide as argument the start value, the intermediate values and the end value, combined with '`:`'. The labels of the scale follow the format used for the start value.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-datapolyscaletitle` *char_string* [Option]
Set the title of the scale relative to the '`-datapolycol real`' data.
Possible values: `any`. Default value: `none`.

`-datafacecol` *char_string* [Option]
Set the colors of the tessellation faces. See option `-datacellcol` for the argument format.
Possible values: `any`. Default value: `white`.

`-datafacecolscheme` *char_string* [Option]
Set the color scheme used to get colors from the data of the tessellation faces loaded with option `-datafacecol`. See option `-datacellcolscheme` for the argument format.
Possible values: `see option -datacellcolscheme`. Default value: `see option -datacellcolscheme`.

`-datafacetrs` *`real`* [Option]
Set the transparency of the tessellation faces. Provide as argument a value that applies to all faces or '`file(`*`file_name`*`)`' to load values from a file.
Possible values: `0 to 1`. Default value: `0`.

`-datafacescale` *`char_string`* [Option]
Set the scale relative to the '`-datafacecol real`' data. Provide as argument the start and end values, combined with '`:`'. To specify the intermediate values, provide as argument the start value, the intermediate values and the end value, combined with '`:`'. The labels of the scale follow the format used for the start value.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-datafacescaletitle` *`char_string`* [Option]
Set the title of the scale relative to the '`-datafacecol real`' data.
Possible values: `any`. Default value: `none`.

`-dataedgerad` *`char_string`* [Option]
Set the radii of the tessellation edges. The argument can be one of the following: a real value that will be used for all entities or '`file(`*`file_name`*`)`' to load values from a file.
Possible values: `any`. Default value: `tessellation dependent`.

`-dataedgecol` *`char_string`* [Option]
Set the colors of the tessellation edges. See option `-datacellcol` for the argument format.
Possible values: `any`. Default value: `black`.

`-dataedgecolscheme` *`char_string`* [Option]
Set the color scheme used to get colors from the data of the tessellation edges loaded with option `-dataedgecol`. See option `-datacellcolscheme` for the argument format.
Possible values: `see option -datacellcolscheme`. Default value: `see option -datacellcolscheme`.

`-dataedgetrs` *`real`* [Option]
Set the transparency of the tessellation edges. Provide as argument a value that applies to all edges or '`file(`*`file_name`*`)`' to load values from a file.
Possible values: `0 to 1`. Default value: `0`.

`-dataedgescale` *`char_string`* [Option]
Set the scale relative to the '`-dataedgecol real`' data. Provide as argument the start and end values, combined with '`:`'. To specify the intermediate values, provide as argument the start value, the intermediate values and the end value, combined with '`:`'. The labels of the scale follow the format used for the start value.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-dataedgescaletitle` *`char_string`* [Option]
Set the title of the scale relative to the '`-dataedgecol real`' data.
Possible values: `any`. Default value: `none`.

`-dataverrad` *`char_string`* [Option]
Set the radii of the tessellation vertices. See option `-dataedgerad` for the argument format.
Possible values: `any`. Default value: `tessellation dependent`.

`-datavercol` *`char_string`* [Option]
Set the colors of the tessellation vertices. See option `-datacellcol` for the argument format.
Possible values: `any`. Default value: `black`.

`-datavercolscheme` *char_string* [Option]
Set the color scheme used to get colors from the data of the tessellation vertices loaded with option `-datavercol`. See option `-datacellcolscheme` for the argument format.
Possible values: `see option -datacellcolscheme`. Default value: `see option -datacellcolscheme`.

`-datavertrs` *real* [Option]
Set the transparency of the tessellation vertices. Provide as argument a value that applies to all vertices or '`file(`*file_name*`)`' to load values from a file.
Possible values: `0 to 1`. Default value: `0`.

`-dataverscale` *char_string* [Option]
Set the scale relative to the '`-datavercol real`' data. Provide as argument the start and end values, combined with '`:`'. To specify the intermediate values, provide as argument the start value, the intermediate values and the end value, combined with '`:`'. The labels of the scale follow the format used for the start value.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-dataverscaletitle` *char_string* [Option]
Set the title of the scale relative to the '`-datavercol real`' data.
Possible values: `any`. Default value: `none`.

`-dataseedrad` *char_string* [Option]
Set the radii of the tessellation seeds. See option `-dataedgerad` for the argument format.
Possible values: `any`. Default value: `tessellation dependent`.

`-dataseedcol` *char_string* [Option]
Set the colors of the tessellation seeds. See option `-datacellcol` for the argument format.
Possible values: `any`. Default value: `gray`.

`-dataseedcolscheme` *char_string* [Option]
Set the color scheme used to get colors from the data of the tessellation seeds loaded with option `-dataseedcol`. See option `-datacellcolscheme` for the argument format.
Possible values: `see option -datacellcolscheme`. Default value: `see option -datacellcolscheme`.

`-dataseedscale` *char_string* [Option]
Set the scale relative to the '`-dataseedcol real`' data. Provide as argument the start and end values, combined with '`:`'. To specify the intermediate values, provide as argument the start value, the intermediate values and the end value, combined with '`:`'. The labels of the scale follow the format used for the start value.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-dataseedscaletitle` *char_string* [Option]
Set the title of the scale relative to the '`-dataseedcol real`' data.
Possible values: `any`. Default value: `none`.

Below are options specific to raster tessellations. For a raster tessellation, it is also possible to set data on a per-voxel basis,

`-datavoxcol` *char_string* [Option]
Set the colors of the voxels, which can be done in two main different ways.
(i) Colors can be specified directly as follows:
• '*value*', where '*value*' can be a color that applies to all cells, or '`file(`*file_name*`)`' for a file containing the individual colors (see Section A.11 [Colors and Color Maps], page 76).

(ii) Colors can be set from data using an argument of the general form '*data_type*:*data_value*', which can be shortened[4] to '*data_value*' in the frequent case where the data type can be unambiguously determined from the data value:
• '`int:`*data_value*' for integer values represented using a color palette, where '*data_value*' can be an integer-value expression such as '`id`' or '`mode`' (see Section A.3 [Raster Tessellation Keys], page 70), or '`file(`*file_name*`)`' for a file containing the individual values.
• '`real:`*data_value*' for real values represented using a smooth color scale, where '*data_value*' can be a real-value expression such as '`x`' or '`vol`' (see Section A.3 [Raster Tessellation Keys], page 70), or '`file(`*file_name*`)`' for a file containing the individual values.
• '`ori:`*data_value*' for the crystal orientations (when applicable), where '*data_value*' can be an orientation (see Section A.9 [Rotations and Orientations], page 75), '`internal`' to use the internal orientations, or '`file(`*file_name*`,[des=`*descriptor*`])`' for a file containing the individual values (see Section A.9 [Rotations and Orientations], page 75). Because '`ori`' is self-defined, '*data_value*' can also be omitted in the case where internal orientations are to be used.
• '`disori:`*data_value*' for the crystal disorientations (the rotation with respect to the nominal cell orientation, when applicable), where '*data_value*' can be a disorientation (see Section A.9 [Rotations and Orientations], page 75), '`internal`' to use the internal disorientations, or '`file(`*file_name*`,[des=`*descriptor*`])`' for a file containing the individual values (see Section A.9 [Rotations and Orientations], page 75). Because '`disori`' is self-defined, '*data_value*' can also be omitted in the case where internal orientations are to be used.
The color schemes used to determine the colors from the data can be fine-tuned using options `-data*colscheme`.
Possible values: `any`. Default value: `white`.

`-datavoxcolscheme` *char_string* [Option]
Set the color scheme used to get colors from the data of the voxels loaded with option `-datavoxcol`. The type of color scheme depends on the type of data.
• For integer values, the color scheme is '`palette`'.
• For real values, the color scheme is '`blue,cyan,yellow,red`' (see Section A.11 [Colors and Color Maps], page 76, for alternatives).
• For crystal orientations (cubic symmetry is assumed) or disorientations (the actual crystal symmetry is assumed), the color scheme can be: '`ipf(`*dir*`)`' for IPF coloring using direction '*dir*', where '*dir*' should be one of '`x`', '`y`' or '`z`' (default '`z`'), '`rodrigues`' for Rodrigues vector coloring (default is inside the fundamental region, can be bounded using '`rodrigues(`*max*`)`', where *max* is the maximum extent), '`axis`' for rotation axis coloring, '`angle`' for rotation angle coloring (can be bounded using '`angle(`*max*`)`', where *max* is the maximum angle (in radian)) and '`axis-angle`' for rotation axis / angle coloring (can be bounded using '`axis-angle(`*max*`)`', where *max* is the maximum angle (in radian)).
Possible values: `see above`. Default value: `"palette" for integer values, "blue,cyan,yellow,red" for real values and "rodrigues" for crystal orientations or disorientations`.

`-datavoxscale` *char_string* [Option]
Set the scale relative to the '`-datavoxcol real`' data. Provide as argument the start and end values, combined with '`:`'. To specify the intermediate values, provide as argument the start value, the intermediate values and the end value, combined with '`:`'. The labels of the scale follow the format used for the start value.
Possible values: `any`. Default value: `data minimum:data maximum`.

[4] This ensures backward compatibility with versions 3.x.

`-datavoxscaletitle` *char_string* [Option]
Set the title of the scale relative to the '`-datavoxcol real`' data.
Possible values: `any`. Default value: `none`.

`-datavoxedgerad` *real* [Option]
Set the radius of the edges of the voxels.
Possible values: `any`. Default value: `proportional to the voxel size`.

`-datavoxedgecol` *char_string* [Option]
Set the color of the edges of the voxels. Provide as argument the name of a color that will be used for all points (see Section A.11 [Colors and Color Maps], page 76).
Possible values: `any`. Default value: `black`.

It is also possible to assign a color to void voxels (i.e., voxels do not belong to any cell). (The edge radius and edge color of void voxels are the same as those of non-void voxels and are set with `-datavoxedgerad` and `-datavoxedgecol`.).

`-datavoidvoxcol` *char_string* [Option]
Set the color of void voxels (see Section A.11 [Colors and Color Maps], page 76).
Possible values: `any`. Default value: `gray`.

5.1.5 Mesh Data Loading and Rendering

The following options enable the definition of the properties (color, size, etc.) of the mesh entities (3D, 2D, 1D and 0D elements, and nodes). This can be done either directly, by specifying the color(s), or indirectly, e.g. from scalar values that are rendered in color using a given *color scheme*. The data can be internal data, data from the simulation directory (if loaded as input), or data loaded from an external file. A scale image is generated in addition to the mesh image. The scale properties can be set up (start and end values, tick values).

The options are listed below for 3D elements ('`elt3d`') and element sets ('`elset3d`'), 2D elements ('`elt2d`') and element sets ('`elset2d`'), 1D elements ('`elt1d`') and element sets ('`elset1d`'), 0D elements ('`elt0d`') and element sets ('`elset0d`'), and nodes ('`nodes`'). Also note that the '*elt*' and '*elset*' labels can be used in place of '`elt`*n*`d`' and '`elset`*n*`d`', where *n* is the highest mesh dimension. This enables the use of the same command whatever the highest mesh dimension is.

The following options enable the loading of data relative to the 3D mesh elements. Note that the options can be applied to element sets by changing '`elt`' to '`elset`'.

`-dataelt3dcol` *char_string* [Option]
Set the colors of the 3D elements, which can be done in two main different ways.
(i) Colors can be specified directly as follows:
• '*value*', where '*value*' can be a color that applies to all elements, or '`file(`*file_name*`)`' for a file containing the individual colors (see Section A.11 [Colors and Color Maps], page 76).
• '`from_nodes`' for colors interpolated from the node colors (defined with `-datanodecol`).
(ii) Colors can be set from data using an argument of the general form '*data_type*`:`*data_value*', which can be shortened[5] to '*data_value*' in the frequent case where the data type can be unambiguously determined from the data value:
• '`int:`*data_value*' for integer values represented using a color palette, where '*data_value*' can be an integer-value expression such as '`id`' or '`mode`' (see Section A.6 [Mesh Keys], page 73), a simulation result (see Section A.8 [Simulation Results], page 75), or '`file(`*file_name*`)`' for a file containing the individual values.
• '`real:`*data_value*' for real values represented using a smooth color scale, where

[5] This ensures backward compatibility with versions 3.x.

'*data_value*' can be a real-value expression such as '`x`' or '`vol`' (see Section A.6 [Mesh Keys], page 73), a simulation result (see Section A.8 [Simulation Results], page 75), or '`file(`*file_name*`)`' for a file containing the individual values.
• '`vector:`*data_value*' for vectorial values (only for VTK output), where '*data_value*' can be a simulation result (see Section A.8 [Simulation Results], page 75) or '`file(`*file_name*`)`' for a file containing the individual values.
• '`tensor:`*data_value*' for tensorial values (only for VTK output), where '*data_value*' can be a simulation result (see Section A.8 [Simulation Results], page 75) or '`file(`*file_name*`)`' for a file containing the individual values. The file can contain either all 9 components or only 6 components, in which case Voigt notation is assumed.
• '`ori:`*data_value*' for the crystal orientations (when applicable), where '*data_value*' can be an orientation (see Section A.9 [Rotations and Orientations], page 75), '`internal`' to use the internal orientations, or '`file(`*file_name*`,[des=`*descriptor*`])`' for a file containing the individual values (see Section A.9 [Rotations and Orientations], page 75). Because '`ori`' is self-defined, '*data_value*' can also be omitted in the case where internal orientations are to be used.
The color schemes used to determine the colors from the data can be fine-tuned using options `-dataelt3dcolscheme`.
Possible values: `any`. Default value: `white`.

`-dataelt3dcolscheme` *char_string* [Option]
Set the color scheme used to get colors from the data of the elements loaded with option `-dataelt3dcol`. The type of color scheme depends on the type of data.
• For integer values, the color scheme is '`palette`'.
• For real values, the color scheme is '`blue,cyan,yellow,red`' (see Section A.11 [Colors and Color Maps], page 76, for alternatives).
• For crystal orientations (cubic symmetry is assumed), the color scheme can be: '`ipf(`*dir*`)`' for IPF coloring using direction '*dir*', where '*dir*' should be one of '`x`', '`y`' or '`z`' (default '`z`'), '`rodrigues`' for Rodrigues vector coloring (default is inside the fundamental region, can be bounded using '`rodrigues(`*max*`)`', where *max* is the maximum extent), '`axis`' for rotation axis coloring, '`angle`' for rotation angle coloring (can be bounded using '`angle(`*max*`)`', where *max* is the maximum angle (in radian)) and '`axis-angle`' for rotation axis / angle coloring (can be bounded using '`axis-angle(`*max*`)`', where *max* is the maximum angle (in radian)).
Possible values: `see above`. Default value: `"palette" for integer values, "blue,cyan,yellow,red" for real values and "rodrigues" for crystal orientations`.

`-dataelt3dscale` *char_string* [Option]
Set the scale relative to the '`-dataelt3dcol real`' data. Provide as argument the start and end values, combined with '`:`'. To specify the intermediate values, provide as argument the start value, the intermediate values and the end value, combined with '`:`'. The labels of the scale follow the format used for the start value.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-dataelt3dscaletitle` *char_string* [Option]
Set the title of the scale relative to the '`-dataelt3dcol real`' data.
Possible values: `any`. Default value: `none`.

`-dataelt3dedgerad` *real* [Option]
Set the radius of the edges of the 3D elements.
Possible values: `any`. Default value: `mesh dependent`.

`-dataelt3dedgecol` *char_string* [Option]
Set the color of the edges of the 3D elements. Provide as argument the name of a color that will be used for all elements (see Section A.11 [Colors and Color Maps], page 76).
Possible values: `any`. Default value: `black`.

The following options enable the loading of data relative to the 2D elements. Note that the options can be applied to element sets by changing '`elt`' to '`elset`'.

`-dataelt2dcol` *char_string* [Option]
Set the colors of the 2D elements. See option `-dataelt3dcol` for the argument format.
Possible values: `any`. Default value: `white`.

`-dataelt2dcolscheme` *char_string* [Option]
Set the color scheme used to get colors from the data of the 2D elements loaded with option `-dataelt2dcol`. See option `-dataelt3dcolscheme` for the argument format.
Possible values: `see option -dataelt3dcolscheme`. Default value: `see option -dataelt3dcolscheme`.

`-dataelt2dscale` *char_string* [Option]
Set the scale relative to the '`-dataelt2dcol real`' data. See option `-dataelt3dscale` for the argument format.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-dataelt2dscaletitle` *char_string* [Option]
Set the title of the scale relative to the '`-dataelt2dcol real`' data.
Possible values: `any`. Default value: `none`.

`-dataelt2dedgerad` *real* [Option]
Set the radius of the edges of the 2D elements.
Possible values: `any`. Default value: `mesh dependent`.

`-dataelt2dedgecol` *char_string* [Option]
Set the colors of the edges of the 3D elements. See option `-dataelt3dedgecol` for the argument format.
Possible values: `any`. Default value: `black`.

The following options enable the loading of data relative to the 1D elements. Note that the options can be applied to element sets by changing '`elt`' to '`elset`'.

`-dataelt1dcol` *char_string* [Option]
Set the colors of the 1D elements. See option `-dataelt3dcol` for the argument format.
Possible values: `any`. Default value: `black`.

`-dataelt1dcolscheme` *char_string* [Option]
Set the color scheme used to get colors from the data of the 1D elements loaded with option `-dataelt1dcol`. See option `-dataelt3dcolscheme` for the argument format.
Possible values: `see option -dataelt3dcolscheme`. Default value: `see option -dataelt3dcolscheme`.

`-dataelt1dscale` *char_string* [Option]
Set the scale relative to the '`-dataelt1dcol real`' data. See option `-dataelt3dscale` for the argument format.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-dataelt1dscaletitle` *char_string* [Option]
Set the title of the scale relative to the '`-dataelt1dcol real`' data.
Possible values: `any`. Default value: `none`.

`-dataelt1drad` *char_string* [Option]
Set the radius of the 1D elements. Provide as argument a value that applies to all elements or '`file(`*file_name*`)`' to load values from a file.
Possible values: `any`. Default value: `mesh dependent`.

The following options enable the loading of data relative to the 0D mesh elements. Note that the options can be applied to element sets by changing '`elt`' to '`elset`'.

`-dataelt0dcol` *char_string* [Option]
Set the colors of the 0D elements. See option `-dataelt3dcol` for the argument format.
Possible values: `any`. Default value: `black`.

`-dataelt0dcolscheme` *char_string* [Option]
Set the color scheme used to get colors from the data of the 0D elements loaded with option `-dataelt0dcol`. See option `-dataelt3dcolscheme` for the argument format.
Possible values: `see option -dataelt3dcolscheme`. Default value: `see option -dataelt3dcolscheme`.

`-dataelt0dscale` *char_string* [Option]
Set the scale relative to the '`-dataelt0dcol real`' data. See option `-dataelt3dscale` for the argument format.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-dataelt0dscaletitle` *char_string* [Option]
Set the title of the scale relative to the '`-dataelt0dcol real`' data.
Possible values: `any`. Default value: `none`.

`-dataelt0drad` *char_string* [Option]
Set the radius of the 1D elements. Provide as argument a value that applies to all elements or '`file(`*file_name*`)`' to load values from a file.
Possible values: `any`. Default value: `mesh dependent`.

The following options enable the loading of data relative to the nodes.

`-datanodecoo` *char_string* [Option]
Set the coordinates of the nodes, which can be done in two main different ways.
(i) Coordinates can be specified directly as follows:
- '*value*', where '*value*' can be '`file(`*file_name*`)`' for a file containing the data.

(ii) Coordinates can be set from data using an argument of the general form '*data_type*`:`*data_value*':
- '`disp:file(`*file_name*`)`' for a file containing the displacement data.
- '`coo`' to load coordinates from the simulation directory and step specified in input.

Possible values: `any`. Default value: `none`.

`-datanodecoofact` *real* [Option]
Set the value of the scaling factor to apply to the displacements of the nodes.
Possible values: `any`. Default value: `1`.

`-datanoderad` *file_name* [Option]
Set the radius of the nodes. Provide as argument a value that applies to all nodes or '`file(`*file_name*`)`' to load values from a file.
Possible values: `any`. Default value: `mesh dependent`.

`-datanodecol` *file_name* [Option]
Set the colors of the nodes. See option `-dataelt3dcol` for the argument format.
Possible values: `any`. Default value: `black`.

`-datanodecolscheme` *char_string* [Option]
Set the color scheme used to get colors from the data of the nodes loaded with option `-datanodecol`. See option `-dataelt3dcolscheme` for the argument format.
Possible values: `see option -dataelt3dcolscheme`. Default value: `see option -dataelt3dcolscheme`.

`-datanodescale` *char_string* [Option]
Set the scale relative to the '`-datanodecol real`' data. See option `-dataelt3dscale` for the argument format.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-datanodescaletitle` *char_string* [Option]
Set the title of the scale relative to the '`-datanodecol real`' data.
Possible values: `any`. Default value: `none`.

5.1.6 Point Data Loading and Rendering

The following options enable the definition of the properties (color, shape, size, etc.) of points loaded as input. This can be done either directly, by specifying the property values (e.g. the RGB channel values for color) or indirectly, e.g. using scalar values that are rendered in color using a given *color scheme*. In this case, a scale image is generated in addition to the image. The scale properties can be set up (start and end values, tick values).

`-datapointcoo` *char_string* [Option]
Set the coordinates of the points. The argument can be of the form '*type*`:file(`*file_name*`)`', where '*type*' can be '`coo`' (for coordinates) or '`disp`' (for displacements), and '*file_name*' is the name of the file containing the data.
Possible values: `any`. Default value: `none`.

`-datapointcoofact` *real* [Option]
Set the value of the scaling factor to apply to the displacements of the points.
Possible values: `any`. Default value: `1`.

`-datapointrad` *char_string* [Option]
Set the radius (and shape) of the points, which can be done using one of the following arguments:
• '`value`', where '*value*' can be a radius that applies to all cells, or '`file(`*file_name*`)`' for a file containing the individual radii.
• '`cube:file(`*file_name*`)`' for cubes of properties defined in '*file_name*'. The file must contain, for each point, the radius (half of the edge length) and the coordinates of the three axes (which also is the rotation matrix that brings the reference axes into coincidence with the cube axes).
• '`cylinder:file(`*file_name*`)`' for cylinders of properties defined in '*file_name*'. The file must contain, for each point, the radius, the length, and the coordinates of the axis.
• '`arr:file(`*file_name*`)`' for arrows of properties defined in '*file_name*'. The file must contain, for each point, the radius, the length, and the coordinates of the axis.

• '`disc:file(`*`file_name`*`)`' for discs of properties defined in '*`file_name`*'. The file must contain, for each point, the radius, and the coordinates of the axis.
• '`ell:file(`*`file_name`*`)`' for ellispoids of properties defined in '*`file_name`*'. The file must contain, for each point, the three radii the coordinates of the three axes.
• '`tor:file(`*`file_name`*`)`' for torus of properties defined in '*`file_name`*'. The file must contain, for each point, the major radius (centre to centre line), the minor radius, and the coordinates of the normal axis.
Possible values: `any`. Default value: `point set dependent`.

`-datapointcol` *`char_string`* [Option]
Set the colors of the points. See option `-dataelt3dcol` for the argument format.
Possible values: `any`. Default value: `gray`.

`-datapointcolscheme` *`char_string`* [Option]
Set the color scheme used to get colors from the data of the points loaded with option `-datapointcol`. See option `-dataelt3dcolscheme` for the argument format.
Possible values: `see option -dataelt3dcolscheme`. Default value: `see option -dataelt3dcolscheme`.

`-datapointtrs` *`real`* [Option]
Set the transparency of the points. Provide as argument a value that applies to all points or '`file(`*`file_name`*`)`' to load values from a file.
Possible values: `0 to 1`. Default value: `0`.

`-datapointedgerad` *`real`* [Option]
Set the radius of the edges of the points.
Possible values: `any`. Default value: `0`.

`-datapointedgecol` *`char_string`* [Option]
Set the color of the edges of the points. Provide as argument the name of a color that will be used for all points (see Section A.11 [Colors and Color Maps], page 76).
Possible values: `any`. Default value: `black`.

`-datapointscale` *`char_string`* [Option]
Set the scale relative to the '`-datapointcol real`' data. See option `-dataelt3dscale` for the argument format.
Possible values: `any`. Default value: `data minimum:data maximum`.

`-datapointscaletitle` *`char_string`* [Option]
Set the title of the scale relative to the '`-datapointcol real`' data.
Possible values: `any`. Default value: `none`.

5.1.7 Coordinate System Rendering

`-datacsyscoo` *`char_string`* [Option]
Set the coordinates of the origin of the coordinate system. Combine the coordinates with '`:`'.
Possible values: `any`. Default value: `0:0:0`.

`-datacsyslength` *`real`* [Option]
Set the length of the coordinate system axes.
Possible values: `any`. Default value: `0.2`.

`-datacsysrad` *`real`* [Option]
Set the radius of the coordinate system axes.
Possible values: `any`. Default value: `0.01`.

`-datacsyslabel` *char_string* [Option]
Set the labels of the coordinate system axes. Combine the labels with '`:`'.
Possible values: `any`. Default value: `X1:X2:X3`.

`-datacsyscol` *char_string* [Option]
Set the color of the coordinate system. Provide as argument any color as detailed in Section A.11 [Colors and Color Maps], page 76.
Possible values: `any`. Default value: `32|32|32`.

5.1.8 Slice Settings

`-slicemesh` *char_string* [Option]
Plot one (or several) slice(s) of the mesh. Provide as argument the equation(s) of the plane(s), under the form '`a*x+b*y+c*z=d`' or any equivalent mathematical expression. Combine with '`,`'.
Possible values: `any`. Default value: `none`.

5.1.9 Show Settings

The following options apply to the full tessellations or mesh.

`-showtess` *logical* [Option]
Show or hide the tessellation.
Possible values: `0` or `1`. Default value: `1 if tess loaded and mesh not loaded, and 0 otherwise`.

`-showtesr` *logical* [Option]
Show or hide the raster tessellation.
Possible values: `0` or `1`. Default value: `1 if tesr loaded and mesh not loaded, and 0 otherwise`.

`-showmesh` *logical* [Option]
Show or hide the mesh.
Possible values: `0` or `1`. Default value: `1 if mesh loaded and slice not loaded, and 0 otherwise`.

`-showmeshslice` *logical* [Option]
Show or hide the mesh slice(s).
Possible values: `0` or `1`. Default value: `1 if slice(s) exist(s) and 0 otherwise`.

`-showpoint` *logical or char_string* [Option]
Show or hide the points. To show only specific points, provide '`file(`*file_name*`)`' to load point numbers from a file.
Possible values: `0` or `1`. Default value: `1 if points exist and 0 otherwise`.

The following option applies to the cells of a tessellation or a raster tessellation, independently of its dimension,

`-showcell` *char_string* [Option]
Specify the cells to show. The argument can be: '`all`' for all, '`none`' for none, '`file(`*file_name*`)`' to load cell identifiers from a file, or any expression based on the keys listed in Section A.2 [Tessellation Keys], page 67, or Section A.3 [Raster Tessellation Keys], page 70.
Possible values: `any`. Default value: `all`.

For a tessellation, it is also possible to set the visibility on a per-entity basis,

`-showpoly` *char_string* [Option]
Specify the polyhedra to show. The argument can be: '`all`' for all, '`none`' for none, '`file(`*file_name*`)`' to load polyhedron identifiers from a file, or any expression based on the keys listed in Section A.2 [Tessellation Keys], page 67.
Possible values: `any`. Default value: `all`.

`-showface` *char_string* [Option]
Specify the faces to show. The argument can be: '`all`' for all, '`none`' for none, '`file(`*file_name*`)`' to load face identifiers from a file, or any expression based on the keys listed in Section A.2 [Tessellation Keys], page 67. The following specific keys are also available: '`cell_shown`' and '`poly_shown`'.
Possible values: `any`. Default value: `none`.

`-showedge` *char_string* [Option]
Specify the edges to show. The argument can be: '`all`' for all, '`none`' for none, '`file(`*file_name*`)`' to load edge numbers from a file, or any expression based on the keys listed in Section A.2 [Tessellation Keys], page 67. The following specific keys are also available: '`cell_shown`', '`poly_shown`' and '`face_shown`'.
Possible values: `any`. Default value: `cell_shown`.

`-showver` *char_string* [Option]
Specify the vertices to show. The argument can be: '`all`' for all, '`none`' for none, '`file(`*file_name*`)`' to load vertex numbers from a file, or any expression based on the keys listed in Section A.2 [Tessellation Keys], page 67. The following specific keys are also available: '`cell_shown`', '`poly_shown`', '`face_shown`' and '`edge_shown`'.
Possible values: `any`. Default value: `none`.

`-showseed` *char_string* [Option]
Specify the seeds to show. The argument can be: '`all`' for all, '`none`' for none, '`file(`*file_name*`)`' to load seed numbers from a file, or any expression based on the keys listed in Section A.2 [Tessellation Keys], page 67. The following specific key is also available: '`cell_shown`'.
Possible values: `any`. Default value: `none`.

`-showfaceinter` *logical* [Secondary option]
Show the interpolations of the tessellation faces (if any). The interpolation edges are printed in gray with a radius equal to the radius of the face edges.
Possible values: `0 or 1`. Default value: `0`.

For a raster tessellation, it is possible to set the visibility of the individual voxels of the tessellation and of the individual voxels that are void (that do not belong to any cell).

`-showvox` *char_string* [Option]
Specify the (non-void) voxels to show. The argument can be: '`all`' for all, '`none`' for none, '`file(`*file_name*`)`' to load voxel identifiers from a file, or any expression based on the keys listed in Section A.3 [Raster Tessellation Keys], page 70.
Possible values: `any`. Default value: `all`.

`-showvoidvox` *char_string* [Option]
Specify the void voxels to show. The argument can be: '`all`' for all, '`none`' for none, '`file(`*file_name*`)`' to load voxel identifiers from a file, or any expression based on the keys listed in Section A.3 [Raster Tessellation Keys], page 70.
Possible values: `any`. Default value: `all`.

The following options apply to the entities of the mesh. The options apply to 3D elements ('`elt3d`') and element sets ('`elset3d`'), 2D elements ('`elt2d`') and element sets ('`elset2d`'), 1D elements ('`elt1d`') and element sets ('`elset1d`'), 0D elements ('`elt0d`') and element sets ('`elset0d`'), and nodes ('`nodes`'). Also note that the '`elt`' and '`elset`' labels can be used in place of '`elt`*`n`*`d`' and '`elset`*`n`*`d`', where *`n`* is the highest mesh dimension. This enables the use of the same command whatever the highest mesh dimension is.

In the following option descriptions, note that any options can be applied to element *sets* by changing '`elt`' to '`elset`'.

`-showelt3d` *`char_string`* [Option]
Specify the 3D elements to show. The argument can be: '`all`' for all, '`none`' for none, '`file(`*`file_name`*`)`' to load element identifiers from a file, or any expression based on the keys listed in Section A.6 [Mesh Keys], page 73.
Possible values: `any`. Default value: `all if highest mesh dim. is 3 and none otherwise`.

`-showelt2d` *`char_string`* [Option]
Specify the 2D elements to show. The argument can be: '`all`' for all, '`none`' for none, '`file(`*`file_name`*`)`' to load element identifiers from a file, or any expression based on the keys listed in Section A.6 [Mesh Keys], page 73. The following specific key is also available: '`elt3d_shown`'.
Possible values: `any`. Default value: `all if highest mesh dim. is 2 and none otherwise`.

`-showelt1d` *`char_string`* [Option]
Specify the 1D elements to show. The argument can be: '`all`' for all , '`none`' for none, '`file(`*`file_name`*`)`' to load element numbers from a file, or any expression based on the keys listed in Section A.6 [Mesh Keys], page 73. The following specific keys are also available: '`elt2d_shown`' and '`elt3d_shown`'.
Possible values: `any`. Default value: `all if highest mesh dim. is 1 and none otherwise`.

`-showelt0d` *`char_string`* [Option]
Specify the 0D elements to show. The argument can be: '`all`' for all '`none`' for none, '`file(`*`file_name`*`)`' to load element numbers from a file, or any expression based on the keys listed in Section A.6 [Mesh Keys], page 73. The following specific keys are also available: '`elt1d_shown`', '`elt2d_shown`' and '`elt3d_shown`'.
Possible values: `any`. Default value: `all if highest mesh dim. is 0 and none otherwise`.

`-shownode` *`char_string`* [Option]
Specify the nodes to show. The argument can be: '`all`' for all , '`none`' for none, '`file(`*`file_name`*`)`' to load node numbers from a file, or any expression based on the keys listed in Section A.6 [Mesh Keys], page 73. The following specific keys are also available: '`elt0d_shown`', '`elt1d_shown`', '`elt2d_shown`' and '`elt3d_shown`'.
Possible values: `any`. Default value: `none`.

`-showcsys` *`logical`* [Option]
Show the coordinate system.
Possible values: `0 or 1`. Default value: `0`.

`-showshadow` *`logical`* [Option]
Show the shadows. If you want colors not affected by shadowing, switch this option off.
Possible values: `0 or 1`. Default value: `1 in 3D and 0 in 2D`.

5.1.10 Camera Settings

`-cameracoo` *char_string:char_string:char_string* [Option]
Specify the camera coordinates. By default, the camera is shifted by *length* times a vector *v* from the centre of the bounding box of the tessellation or mesh. The variable *length* is the average length of the bounding box (1 for a unit cube), and the coordinates of vector *v* are denoted as *vx*, *vy* and *vz* (= 3.462, -5.770 and 4.327, respectively, in 3D, and 0, 0 and 8, respectively, in 2D). The coordinates of the tessellation or mesh centre are denoted as *x*, *y* and *z* (if both a tessellation and a mesh have been loaded, the mesh is considered). Provide as argument the expression for the 3 coordinates, combined with '`:`'.
Possible values: `any`. Default value: `x+length*vx:y+length*vy:z+length*vz`.

`-cameralookat` *char_string:char_string:char_string* [Option]
Specify the camera look-at point. By default, the point is the tessellation or mesh centre. The coordinates of the tessellation or mesh centre are denoted as *x*, *y* and *z* (if both a tessellation and a mesh have been loaded, the mesh is considered). Provide as argument the expression for the 3 coordinates, combined with '`:`'.
Possible values: `any`. Default value: `x:y:z`.

`-cameraangle` *real* [Option]
Specify the opening angle of the camera along the horizontal direction (in degrees). The opening angle along the vertical direction is determined from the opening along the horizontal direction and the image size ratio.
Possible values: `any`. Default value: `25`.

`-camerasky` *real:real:real* [Option]
Specify the sky vector of the camera (vertical direction). Provide as argument the coordinates combined with '`:`'.
Possible values: `any`. Default value: `0:1:0 in 2D and 0:0:1 in 3D`.

`-cameraprojection` *char_string* [Option]
Specify the type of projection of the camera.
Possible values: `perspective or orthographic`. Default value: `perspective for 3D and orthographic for 2D`.

5.1.11 Output Image Settings

`-imagesize` *int:int* [Option]
Specify the size of the image (in pixels). Provide as argument the width and height, combined with '`:`'.
Possible values: `any`. Default value: `1200:900`.

`-imagebackground` *char_string* [Option]
Specify the color of the background. Provide as argument any color as detailed in Section A.11 [Colors and Color Maps], page 76.
Possible values: `any`. Default value: `white`.

`-imageantialias` *logical* [Option]
Use antialiasing to produce a smoother image. Switch antialiasing off for faster image generation or smaller image file.
Possible values: `0 or 1`. Default value: `1`.

`-imageformat` *char_string* [Option]
Specify the output image format. It can be the PNG format (`png`), the POV-Ray format (`pov`) or the VTK format (`vtk`). Use '`pov:objects`' to get a POV-Ray file con-

taining only the objects[6]. Combine with '`,`'.
Possible values: `see above`. Default value: `png`.

5.1.12 Scripting

`-loop char_string real real real ... -endloop` [Option]
Create a loop of commands. Provide as argument the name of the loop variable, its initial value, the loop increment value, the final value, and the commands to execute. An example of use of the `-loop` / `-endloop` capability is provided in the Examples Section.
Possible values: `any`. Default value: `none`.

5.1.13 Output Options

`-outdir char_string,char_string,...` [Option]
Use this option to set the output directory. Provide the directory name, or '`sim_dir`' to use the dedicated location of the simulation directory, *`dir.sim`*`/images/`*`format`*, where *`format`* is the image format (see option `-imageformat`). '`sim_dir`' applies only if a simulation directory is loaded as input. Several values can be combined with '`,`', in which case the first valid value is used. (To write to a simulation directory when loaded as input and to the local directory otherwise, use '`sim_dir,.`'[7].)
Possible values: `any`. Default value: `"."`.

5.1.14 Print Options

`-print char_string` [Option]
Use this option to print the image. Provide as argument the file name, excluding its extension.
Possible values: `any`. Default value: `none`.

5.1.15 Advanced Options

`-includepov char_string:char_string:...` [Option]
Use this option to include additional objects to the image, under the form of a POV-Ray file. Provide as first argument the name of the POV-Ray file and as next arguments successive transformations to apply to the objects of the POV-Ray file. The transformations can be '`translate(`*`vx`*`,`*`vy`*`,`*`vz`*`)`' for a translation of vector (vx, vy, vz), '`scale(`*`sx`*`,`*`sy`*`,`*`sz`*`)`' for scaling by factors sx, sy and sz in the three directions of space, and '`rotate(`*`thetax`*`,`*`thetay`*`,`*`thetaz`*`)`' for a rotation of angles *thetax*, *thetay* and *thetaz* about axes x, y and z[8].
Possible values: `any`. Default value: `none`.

5.2 Output Files

The output files are

- PNG file, `.png`: a bitmapped image (the alpha channel is off).

[6] Not compatible with '`png`'; the resulting file can be loaded with `-includepov`.

[7] This may be written to the initialization file.

[8] The rotation is read in POV-Ray style; i.e., according to the POV-Ray documentation: *Note that the order of the rotations does matter. Rotations occur about the x-axis first, then the y-axis, then the z-axis. If you are not sure if this is what you want then you should only rotate on one axis at a time using multiple rotation statements to get a correct rotation. Rotation is always performed relative to the axis. Thus if an object is some distance from the axis of rotation it will not only rotate but it will orbit about the axis as though it was swinging around on an invisible string. POV-Ray uses a left-handed rotation system. Using the famous "Computer Graphics Aerobics" exercise, you hold up your left hand and point your thumb in the positive direction of the axis of rotation. Your fingers will curl in the positive direction of rotation. Similarly if you point your thumb in the negative direction of the axis your fingers will curl in the negative direction of rotation.*

- POV-Ray file, `.pov`: a POV-Ray script file.
- VTK file, `.vtk`: a VTK file, for interactive visualization.

A PNG image can be obtained from a POV-Ray file by invoking POV-Ray as follows (see the POV-Ray documentation for details and further commands), `povray` *`file.pov`* `+W`*`image_width`* `+H`*`image_height`* `-D +A0.2`.

5.3 Examples

Below are some examples of use of neper -V.

1. Print out tessellation `n10-id1.tess` with cells colored from their identifiers and an image size of 900×450 pixels.
```
$ neper -V n10-id1.tess -datacellcol id -imagesize 900:450 -print img
```
2. Print out tessellation `n10-id1.tess` with cells colored from crystal orientations and semi-transparency.
```
$ neper -V n10-id1.tess -datacellcol ori -datacelltrs 0.5 -print img
```
3. Print out mesh `n10-id1.msh` with elements colored from scalar values written in file `v` and a scale ranging from 0 to 100.
```
$ neper -V n10-id1.msh -dataeltcol "real:file(v)" -dataeltscale 0:100 \
        -print img
```
4. Print out mesh `n10-id1.msh` with elements colored from nodal scalar values written in file `v` and a scale ranging from 0 to 100.
```
$ neper -V n10-id1.msh -datanodecol "real:file(v)" -dataeltcol \
        from_nodes -dataeltscale 0:100 -print img
```
5. Print out the 10 first cells of a 100-cell tessellation, colored from their identifiers and semi-transparency, and with edges shown in red and vertices shown as green spheres of radius 0.01.
```
$ neper -V n100-id1.tess -showcell "id<=10" \
        -datacellcol id -datacelltrs 0.5 \
        -showedge cell_shown -showver cell_shown \
        -dataverrad 0.01 -dataedgecol red -datavercol green \
        -print img
```
6. Print out the interior element sets of mesh `n100-id1.msh` and show the 1D elements.
```
$ neper -V n100-id1.tess,n100-id1.msh -dataelsetcol id \
        -showelset 'body>0' -showelt1d elt3d_shown -print img
```
7. Print out 3 slices of mesh `n100-id1.msh`.
```
$ neper -V n100-id1.msh -dataelsetcol id \
        -slicemesh "x=0.5,y=0.5,z=0.5" -print img
```
8. Print out slices of mesh `n100-id1.msh`, at z coordinates ranging from 0.1 to 0.9 by step of 0.1, each slice being printed in a separate file.
```
$ neper -V n100-id1.msh -dataelsetcol id \
        -loop Z 0.1 0.1 0.9 \
        -slicemesh "z=Z" -print imgZ \
        -endloop
```
9. Print out a deformed mesh colored by orientations, defined from a simulation directory.
```
$ neper -V mysim.sim -simstep 10 -datanodecoo coo \
        -dataeltcol ori -print img
```

10. Print out a deformed mesh colored by orientations, defined from a simulation directory; generate an image at each deformation step.

```
$ neper -V mysim.sim -loop STEP 0 1 10 -simstep STEP -datanodecoo coo \
        -dataeltcol ori -print imgSTEP -endloop
```

Appendix A Expressions and Keys

A.1 Mathematical and Logical Expressions

Neper handles mathematical expressions thanks to the `muparser` library. The expression must contain no space, tabulation or new-line characters, and match the following syntax[1].

A.1.1 Functions

The following table gives an overview of the functions supported by the default implementation. It lists the function names, the number of arguments and a brief description.

Name	**Description**
`sin`	sine function
`cos`	cosine function
`tan`	tangens function
`asin`	arcus sine function
`acos`	arcus cosine function
`atan`	arcus tangens function
`sinh`	hyperbolic sine function
`cosh`	hyperbolic cosine
`tanh`	hyperbolic tangens function
`asinh`	hyperbolic arcus sine function
`acosh`	hyperbolic arcus tangens function
`atanh`	hyperbolic arcur tangens function
`log2`	logarithm to the base 2
`log10`	logarithm to the base 10
`log`	logarithm to the base 10
`ln`	logarithm to base e (2.71828...)
`exp`	e raised to the power of x
`sqrt`	square root of a value
`sign`	sign function: -1 if $x < 0$; 1 if $x > 0$
`rint`	round to nearest integer
`abs`	absolute value
`min`	min of all arguments
`max`	max of all arguments
`sum`	sum of all arguments
`avg`	mean value of all arguments

A.1.2 Binary Operators

The following table lists the default binary operators supported by the parser.

Operator	**Description**	**Priority**
`&&`	logical and	1
`||`	logical or	2
`<=`	less or equal	4
`>=`	greater or equal	4
`!=`	not equal	4
`==`	equal	4

[1] Taken from the `muparser` documentation, see `http://beltoforion.de/article.php?a=muparser` for more information.

`>`	greater than	4
`<`	less than	4
`+`	addition	5
`-`	subtraction	5
`*`	multiplication	6
`/`	division	6
`^`	raise x to the power of y	7

A.1.3 Ternary Operators

The parser has built in support for the if-then-else operator. It uses lazy evaluation in order to make sure only the necessary branch of the expression is evaluated.

Operator	**Description**
`?:`	if-then-else operator, following the C/C++ syntax: `(test)?value_if_true:value_if_false`.

A.1.4 Statistical Distributions

The following table lists the statistical distributions. Arguments enclosed in square brackets ('`[`' and '`]`') are optional. Custom endpoints (not indicated) can also be added as arguments, as described in the following.

Operator	**Description**	**Information**
`normal(`*mean*`,`*sigma*`)`	normal	
`lognormal(`*mean*`,`*sigma*`)`	lognormal	
`dirac(`*mean*`)`	Dirac	
`beta(`*x*`,`*y*`)`	beta function	$x > 0$, $y > 0$
`lorentzian(`*mean*`,`*sigma*`)`	Lorentzian	
`studentst(`*mean*`,`*sigma*`)`	Student's t	
`weibull(`*k*`,`*sigma*`)`	Weibull	$k > 0$ represents the shape
`breitwigner(`*mean*`,`*sigma*`[,`*gamma*`])`	Breit-Wigner	$gamma \geq 0$, default 1
`expnormal(`*mean*`,`*sigma*`[,`*gamma*`])`	exp-normal	$gamma > 0$ default $sigma$
`moffat(`*mean*`,`*sigma*`[,`*gamma*`])`	Moffat	$gamma > 0$, default 1
`pearson7(`*mean*`,`*sigma*`[,`*gamma*`])`	Pearson type VII	default $gamma = 1.5$
`pseudovoigt(`*mean*`,`*sigma*`[,`*gamma*`])`	Pseudo-Voigt	$gamma \in [0, 1]$, default 0.5
`skewnormal(`*mean*`,`*sigma*`[,`*gamma*`])`	skewed normal	default $gamma = sigma$

'`mean`' represents the mean (or centre), and '`sigma`' (> 0) represents the standard deviation (or scale). '`gamma`' depends on the distribution function (see the above table). For all distributions, custom endpoints can be added as last arguments, '*`from`*`,`*`to`*', where '*`from`*' is the lower end point and '*`to`*' is the upper endpoint. If the parameter keywords are used, the parameters can be given in any order; e.g., '`moffat(`*gamma*`=1,`*from*`=0,`*to*`=1,`*sigma*`=0.1,`*mean*`=0.5)`'. Otherwise, the parameters are read based on their positions; e.g., '`lognormal(0.25,0.01)`' yields $mean = 0.25$ and $sigma = 0.01$. It is also possible (but not recommended) to specify some variables by keyword and let others be read by position. Endpoints are considered inclusive by default, but exclusive endpoints can be specified using '`fromexclusive=`*from*' and '`toexclusive=`*to*' ('`frominclusive=`*from*' and '`toinclusive=`*to*' can be used for inclusive endpoints). String completion is available for the keywords. Finally, a sum of distributions of increasing averages can be provided; e.g., '`0.3*lognormal(0.5,0.1)+0.7*normal(1,0.1)`'.

A.2 Tessellation Keys

Available keys for a tessellation itself are provided below.

Key	Descriptor	Apply to
`dim`	dimension	tess
`vernb`	number of vertices	tess
`edgenb`	number of edges	tess
`facenb`	number of faces	tess
`polynb`	number of polyhedra	tess
`cellnb`	number of cells	tess
`x`	x coordinate	tess
`y`	y coordinate	tess
`z`	z coordinate	tess
`coo`	x, y and z coordinates	tess
`area`	area	tess
`vol`	volume	tess
`size`	size (area/volume in 2D/3D)	tess

Available keys for tessellation seeds, vertices, edges, faces and polyhedra are provided below. Also note that the descriptors apply to *cells* if they are tagged to apply to *polyhedra* and the tessellation is 3D and *faces* and the tessellation is 2D. You may also replace, in the tessellation keys themselves, '`face`' by '`cell`' if the tessellation is 2D and '`poly`' by '`cell`' if the tessellation is 3D (it applies only on rare occasions). For example, for a 2D tessellation, you may use `-statcell ncells` instead of `-statface nfaces`. Keys specific to cells are defined accordingly in the following but also apply to *faces* is the tessellations is 2D and *polys* is the tessellation is 3D.

To turn a key value into a value relative to the mean over all entities (e.g. the relative cell size), append the key expression with the '`:rel`' modifier. To turn a key value into a value which holds for a unit cell size, append the key expression with the '`:uc`' modifier. To use as a reference only the *body* or *true* entities (see below), append '`b`' or '`t`' to the modifiers, respectively.

Key	Descriptor	Apply to
`dim`	dimension	tess
`vernb`	number of vertices	tess
`edgenb`	number of edges	tess
`facenb`	number of faces	tess
`polynb`	number of polyhedra	tess
`cellnb`	number of cells	tess
`vernb`	number of vertices	tess
`id`	identifier	seed, ver, edge, face, poly
`x`	x coordinate	tess, seed, ver, edge, face, poly
`y`	y coordinate	tess, seed, ver, edge, face, poly
`z`	z coordinate	tess, seed, ver, edge, face, poly
`coo`	x, y and z coordinates	tess, seed, ver, edge, face, poly
`xmin`	minimum x coordinate	edge, face, poly
`ymin`	minimum y coordinate	edge, face, poly
`zmin`	minimum z coordinate	edge, face, poly
`xmax`	maximum x coordinate	edge, face, poly
`ymax`	maximum y coordinate	edge, face, poly
`zmax`	maximum z coordinate	edge, face, poly

`w`	weight (width for a lamella tessellation)	seed, cell
`true`	true level	ver, edge, face, poly
`body`	body level	ver, edge, face, poly
`state`	state	ver, edge, face, poly
`domtype`	type of domain (0 if on a domain vertex, 1 if on a domain edge and 2 if on a domain face)	ver, edge, face
`domface`	domain face (-1 if undefined)	face
`domedge`	domain edge (-1 if undefined)	edge
`domver`	domain vertex (-1 if undefined)	ver
`scale`	scale	face[2]
`length`	length	edge
`area`	area	tess, face, poly
`vol`	volume	tess, poly
`size`	size (area/volume in 2D/3D)	tess, cell
`diameq`	equivalent diameter[3]	tess, face, poly
`radeq`	equivalent radius[4]	tess, face, poly
`sphericity`	sphericity[5]	poly
`circularity`	circularity[6] (2D counterpart of sphericity)	face
`convexity`	convexity[7]	face[8], poly
`dihangleav`	average dihedral angle	face, poly
`dihanglemin`	minimum dihedral angle	face, poly
`dihanglemax`	maximum dihedral angle	face, poly
`dihangles`	dihedral angles	face, poly
`ff`	flatness fault (in degrees)	face
`theta`	disorientation angle (in degrees)	edge (in 2D), face (in 3D)
`cyl`	whether or not is used to describe the circular part of a cylinder domain	edge
`vernb`	number of vertices	edge, face, poly
`vers`	vertices	edge, face, poly
`edgenb`	number of edges	ver, face, poly
`edges`	edges	ver, face, poly
`facenb`	number of faces	ver, edge, poly
`faces`	faces	ver, edge, poly
`polynb`	number of polyhedra	ver, edge, face
`polys`	polyhedra	ver, edge, face
`nfacenb`	number of neighboring faces	face
`nfaces`	neighboring faces	face

[2] Applies only to a 3D tessellation and relevant for multiscale tessellations. The scale of a face is the scale at which the face was created, and it ranges from 0 (for domain faces) to the number of scales of the tessellation (for the last created faces).

[3] Equivalent diameter = diameter of the circle of equivalent area/volume in 2D/3D.

[4] Equivalent radius = radius of the circle of equivalent area/volume in 2D/3D.

[5] Sphericity of a polyhedron = ratio of the surface area of the sphere of equivalent volume to the surface area of the polyhedron.

[6] Circularity of a polygon = ratio of the perimeter of the circle of equivalent area to the perimeter of the polygon.

[7] Convexity of a polyhedron (face) = ratio of the volume (area) of the polyhedron (face) to the volume (area) of the convex hull of the polyhedron (face).

[8] Applies only to a 2D tessellation.

`nfacenb_samedomain`	number of neighboring faces of the same domain (parent cell of a multiscale tessellation)	face (in 2D)
`nfaces_samedomain`	neighboring faces of the same domain (parent cell of a multiscale tessellation)	face (in 2D)
`npolynb`	number of neighboring polyhedra	poly
`npolys`	neighboring polyhedra	poly
`npolynb_samedomain`	number of neighboring polyhedra of the same domain (parent cell of a multiscale tessellation)	poly
`npolys_samedomain`	neighboring polyhedra of the same domain (parent cell of a multiscale tessellation)	poly
`vercoos`	vertex coordinates	face, poly
`faceareas`	face surface areas	poly
`faceeqs`	face equations[9]	poly
`nseednb`	number of neighboring seeds	poly
`nseeds`	neighboring seeds[10]	poly
`scaleid(`*`scale`*`)`	identifier of the corresponding cell at scale *scale*	cell
`lam`	lamella width id[11]	cell
`mode`	mode[12]	cell
`group`	group	cell
`per`	periodic (1 if periodic, 0 otherwise)	ver, edge, face (in 3D)

Variables consisting of several values ('`vers`', etc.) are not available for sorting (option `-sort`).

For a cell, the `body` and `true` variables are defined as follows,

- ***`body`*** is an integer equal to `0` if the cell is at the domain boundary, i.e. if it shares at least one face with it (edge in 2D), and is equal to `1` or higher otherwise. This is determined as follows: if a cell is surrounded by cells with ***`body`*** values equal to or higher than ***`n`***, its ***`body`*** value is equal to ***`n`*** `+ 1`. Therefore, `body` tends to increase with the distance to the domain boundary and can be used to define cells that may suffer from boundary effects.
- ***`true`*** is an integer equal to `0` it the cell shape is biased by the domain boundary, and is equal to `1` or higher otherwise. A value higher than `0` is achieved if and only if any seed that would have been located outside the domain (where it could not be) would not have affected the shape of the cell. This condition is fulfilled if the distance between the seed of the cell and any of its vertices is lower than the minimum distance between a vertex of the cell and the domain boundary. ***`true`*** is extended to values higher than `1` in the same way as body: if a cell is surrounded by cells with ***`true`*** values equal to or higher than ***`n`***, its ***`true`*** value is equal to ***`n`*** `+ 1`. As ***`body`***, ***`true`*** tends to increase with the distance to the domain boundary, and $true \leq body$. ***`true`*** is especially useful for statistics on the cells (morphology, mesh, etc.), for which only cells with $true \geq 1$ should be considered.

For entities of lower dimension than cells (vertices, edges and faces), ***`body`*** and ***`true`*** are equal to the maximum ***`body`*** or ***`true`*** values of the cells they belong to.

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[9] A face equation is specified by the parameters d, a, b and c, with the equation being: $ax + by + cz = d$. The vector (a, b, c) is pointing outwards of the polyhedron.

[10] If a polyhedron has no neighbor on a face, a negative value is returned.

[11] In the case of a lamellar tessellation with several lamella widths, *lam* stands for the actual lamella width of the cell (starting from 1).

[12] In the case of a multimodal tessellation (e.g. in terms of cell size), *mode* stands for the actual mode (starting from 1).

A.3 Raster Tessellation Keys

Available keys for raster tessellation itself are provided below.

Key	Descriptor	Apply to
`dim`	dimension	tesr
`voxnbx`	number of voxels in direction x	tesr
`voxnby`	number of voxels in direction y	tesr
`voxnbz`	number of voxels in direction z	tesr
`voxnb`	number of voxels in total	tesr
`originx`	origin x coordinate	tesr
`originy`	origin y coordinate	tesr
`originz`	origin z coordinate	tesr
`voxsizex`	voxel size in direction x	tesr
`voxsizey`	voxel size in direction y	tesr
`voxsizez`	voxel size in direction z	tesr
`domsizex`	domain size in direction x	tesr
`domsizey`	domain size in direction y	tesr
`domsizez`	domain size in direction z	tesr
`x`	x coordinate	tesr
`y`	y coordinate	tesr
`z`	z coordinate	tesr
`coo`	x, y and z coordinates	tesr

Available keys for raster tessellation seeds, cells and voxels are provided below. Mathematical and logical expressions based on these keys can also be used. To turn a key value into a value relative to the mean over all entities (e.g. the relative cell size), append the key expression with the '`:rel`' modifier. To turn a key value into a value which holds for a unit cell size, append the key expression with the '`:uc`' modifier.

Key	Descriptor	Apply to
`originx`	origin x coordinate	tesr
`originy`	origin y coordinate	tesr
`originz`	origin z coordinate	tesr
`voxsizex`	voxel size in direction x	tesr
`voxsizey`	voxel size in direction y	tesr
`voxsizez`	voxel size in direction z	tesr
`domsizex`	domain size in direction x	tesr
`domsizey`	domain size in direction y	tesr
`domsizez`	domain size in direction z	tesr
`id`	identifier	seed, cell, voxel
`x`	x coordinate	tesr, seed, cell, voxel
`y`	y coordinate	tesr, seed, cell, voxel
`z`	z coordinate	tesr, seed, cell, voxel
`coo`	x, y and z coordinates	tesr, seed, cell, voxel
`vx`	x coordinate (in voxel)	voxel
`vy`	y coordinate (in voxel)	voxel
`vz`	z coordinate (in voxel)	voxel
`vcoo`	x, y and z coordinates (in voxel)	voxel
`cell`	cell	voxel
`w`	Laguerre weight	seed
`size`	size (area/volume in 2D/3D)	cell

`diameq`	equivalent diameter[13]	cell
`radeq`	equivalent radius[14]	cell
`convexity`	convexity[15]	cell

A.4 Tessellation Optimization Keys

A.4.1 Time Keys

The available keys for option `-morphooptilogtime` are provided below. Use '`iter(`*`factor`*`)`', where '*`factor`*' is an integer reduction factor, to log values only at specific iteration numbers.

Key	**Descriptor**
`iter`	iteration number
`varupdateqty`	number of updated variables
`seedupdateqty`	number of updated seeds
`seedupdatelist`	list of updated seeds
`cellupdateqty`	number of updated cells
`cellupdatelist`	list of updated cells
`var`	time for variable update
`seed`	time for seed update
`cell_init`	time for cell update initialization
`cell_kdtree`	time for cell update kdtree computation
`cell_shift`	time for cell update shift computation
`cell_neigh`	time for cell update neigh. computation
`cell_cell`	time for cell update cell computation
`cell_other`	time for cell update others
`cell_total`	total time for cell update
`val`	time for (objective function) value update
`val_init`	time for (objective function) value update / initialization
`val_penalty`	time for (objective function) value update / penalty computation
`val_val`	time for (objective function) value update / value computation
`val_val_cellval`	time for (objective function) value update / value computation / cell values
`val_val_comp`	time for (objective function) value update / value computation / computation
`val_comp`	time for (objective function) value update / computation
`total`	total time
`cumtotal`	cumulative total time

A.4.2 Variable Keys

The available keys for option `-morphooptilogvar` are provided below. Use '`iter(`*`factor`*`)`', where '*`factor`*' is an integer reduction factor, to log values only at specific iteration numbers.

Key	**Descriptor**	**Apply to**
`iter`	iteration number	n/a
`id`	identifier	seed
`x`	x coordinate	seed
`y`	y coordinate	seed

[13] Equivalent diameter = diameter of the circle of equivalent area/volume in 2D/3D.

[14] Equivalent radius = radius of the circle of equivalent area/volume in 2D/3D.

[15] Convexity of a cell = ratio of the volume of the cell to the volume of the convex hull of the cell.

`z`	z coordinate	seed
`w`	weight	seed

A.4.3 Objective Function Value Keys

The available keys for option `-morphooptilogval` are provided below. Use '`iter(factor)`', where '*`factor`*' is an integer reduction factor, to log values only at specific iteration numbers.

Key	**Descriptor**	**Apply to**
`iter`	iteration number	n/a
`val`	value	n/a
`valmin`	minimal value	n/a
`val0`	value, without smoothing	n/a
`valmin0`	minimal value, without smoothing	n/a
`val(i)`	*i*th subvalue	n/a
`val0(i)`	*i*th subvalue, without smoothing	n/a
`eps`	error on the objective function (see option `-morphooptistop`)	n/a
`reps`	relative error on the objective function (see option `-morphooptistop`)	n/a
`loop`	optimization loop	n/a
`plateaulength`	current plateau length[16]	n/a

A.4.4 Statistical Distribution Keys

The available keys for option `-morphooptilogdis` are provided below. PDF stands for *probability density function* and CDF stands for *cumulative probability density function*. Use '`iter(factor)`', where '*`factor`*' is a reduction factor, to log values only at specific iteration numbers.

Key	**Descriptor**	**Apply to**
`iter`	iteration number	n/a
`x`	x coordinate	n/a
`tarpdf`	target PDF	n/a
`tarcdf`	target CDF	n/a
`curpdf`	current PDF	n/a
`curcdf`	current CDF	n/a
`tarpdf0`	target PDF, not smoothed	n/a
`tarcdf0`	target CDF, not smoothed	n/a
`curcdf0`	current CDF, not smoothed	n/a

A.4.5 Raster Tessellation Voxel Keys

The available keys for option `-morphooptilogtesr` are provided below. Values are written for each voxel used to compute the objective function. Use '`iter(factor)`', where '*`factor`*' is a reduction factor, to log values only at specific iteration numbers.

Key	**Descriptor**	**Apply to**
`iter`	iteration number	n/a
`id`	cell identifier	n/a
`x`	x coordinate	n/a
`y`	y coordinate	n/a

[16] Number of iterations during which the objective function did not decrease.

`z`	z coordinate	n/a
`dist`	distance to the cell	n/a

A.5 Orientation Optimization Keys

A.5.1 Variable Keys

The available keys for option `-orioptilogvar` are provided below. For all orientation descriptors but '`quaternion`', the returned orientation are located in the fundamental region.

Key	**Descriptor**	**Apply to**
`iter`	iteration number	n/a
`id`	identifier	seed
`rodrigues`	Rodrigues vector	seed
`euler-bunge`	Euler angles (Bunge convention)	seed
`euler-kocks`	Euler angles (Kocks convention)	seed
`euler-roe`	Euler angles (Roe convention)	seed
`rotmat`	rotation matrix	seed
`axis-angle`	rotation axis / angle pair	seed
`quaternion`	quaternion	seed

A.6 Mesh Keys

Available keys for a mesh itself are provided below.

Key	**Descriptor**	**Apply to**
`eltnb`	element number	*n*D mesh, cohesive-elt mesh
`nodenb`	node number	*n*D mesh
`partnb`	partition number	highest-dimension mesh
`x`	x coordinate	*n*D mesh
`y`	y coordinate	*n*D mesh
`z`	z coordinate	*n*D mesh
`coo`	x, y and z coordinates	*n*D mesh
`length`	length	1D mesh
`area`	area	2D mesh
`vol`	volume	3D mesh
`size`	size (length/area/volume in 1D/2D/3D)	1D mesh, 2D mesh, 3D mesh

Available keys for mesh node, elements and element sets (of all dimensions) and points are provided below.

Key	**Descriptor**	**Apply to**
`id`	identifier	node, *n*D elt, *n*D elset
`x`	x coordinate	node, *n*D elt, *n*D elset
`y`	y coordinate	node, *n*D elt, *n*D elset
`z`	z coordinate	node, *n*D elt, *n*D elset
`coo`	x, y and z coordinates	node, *n*D elt, *n*D elset
`dim`	dimension (= lowest parent elt dimension)	node
`elset0d`	0D elset	0D elt
`elset1d`	1D elset	1D elt

`elset2d`	2D elset	2D elt
`elset3d`	3D elset	3D elt
`part`	partition	nD elt, node
`group`	group	nD elt, nD elset
`cyl`	whether or not is used to describe the circular part of a cylinder domain	1D elt, 1D elset
`vol`	volume	3D elt, 3D elset
`area`	area	2D elt
`diameq`	equivalent diameter[17]	2D elt, 3D elt, 2D elset, 3D elset
`radeq`	equivalent radius[18]	2D elt, 3D elt, 2D elset, 3D elset
`length`	average edge length	nD elt, 1D elset
`lengths`	edge lengths	2D elt, 3D elt
`elsetvol`	elset volume	3D elt
`elsetarea`	elset area	2D elt
`elsetlength`	elset length	1D elt
`rr`	radius ratio	3D elt
`rrav`, `rrmin`, `rrmax`	average, min and max radius ratios	3D elset
`Osize`	Osize	3D elset
`eltnb`	number of elements	nD elset
`true`	true level	nD elt, nD elset
`body`	body level	nD elt, nD elset
`domtype`	type of domain (0 if on a domain vertex, 1 if on a domain edge and 2 if on a domain face)	2D elset, 1D elset, 0D elset, 2D elt, 1D elt, 0D elt
`2dmeshp`	coordinates of the closest point of the 2D mesh	node, 3D elt
`2dmeshd`	distance to '`2dmeshp`'	node, 3D elt
`2dmeshv`	vector to '`2dmeshp`'	node, 3D elt
`2dmeshn`	outgoing normal vector of the 2D mesh at '`2dmeshp`'	node, 3D elt
`per`	periodic (1 if periodic, 0 otherwise)	0D elt, 1D elt, 2D elt (in 3D), 0D elset, 1D elset, 2D elset (in 3D)
`col_rodrigues`	color according to the Rodrigues vector color convention[19]	node
`col_stdtriangle`	color according to the stereographic triangle (IPF) color convention[20]	node

nD stands for an arbitrary dimension (from 0D to 3D). Variables beginning with '`2dmesh`' are only available for statistics (options beginning with `-stat` of module -M); for elements, they apply to the centroids.

A.7 Point Keys

Available keys for points are provided below.

[17] Equivalent diameter = diameter of the circle of equivalent area/volume in 2D/3D.

[18] Equivalent radius = radius of the circle of equivalent area/volume in 2D/3D.

[19] Applies to a mesh of Rodrigues space.

[20] Applies to a mesh of the stereographic triangle.

Key	Descriptor	Apply to	Require
`id`	identifier	point	
`x`	x coordinate	point	
`y`	y coordinate	point	
`z`	z coordinate	point	
`cell`	cell	point	tessellation
`elt`	containing element	point	mesh
`elset`	containing elset	point	mesh
`2dmeshp`	coordinates of the closest point of the 2D mesh	point	3D mesh
`2dmeshd`	distance to '`2dmeshp`'	point	3D mesh
`2dmeshv`	vector to '`2dmeshp`'	point	3D mesh
`2dmeshn`	outgoing normal vector of the 2D mesh at '`2dmeshp`'	point	3D mesh

A.8 Simulation Results

A result of the simulation directory can be invoked simply from its name (see Section B.6 [Simulation Directory (`.sim`)], page 92). A component of a vectorial or tensorial result can be invoked by prefixing the component to the name, as in `coo1`, `stress11`, etc. For a symmetrical tensor, both *`tij`* and *`tji`* are valid. The type of a result of the simulation directory is determined automatically.

A.9 Rotations and Orientations

Rotations and orientations can be described using the following descriptors.

Key	Descriptor	Number of parameters
`rodrigues`	Rodrigues vector	3
`euler-bunge`	Euler angles (Bunge convention)	3
`euler-kocks`	Euler angles (Kocks convention)	3
`euler-roe`	Euler angles (Roe convention)	3
`rotmat`	rotation matrix	9
`axis-angle`	rotation axis / angle pair	4
`quaternion`	quaternion	4

Some options can take orientations as argument, in which case the orientation must be expressed as '*`descriptor(parameters)`*', where the parameters are separated by '`,`', such as '`rodrigues(0.1,0.2,0.3`').

Keys are available for ideal orientations (lowercased is accepted):

Cube	$(0\,0\,1)\,[1\,0\,0]$
Goss	$(0\,1\,1)\,[1\,0\,0]$
U	$(1\,0\,1)\,[\bar{1}\,0\,1]$
45NDCube	$(0\,0\,1)\,[1\,\bar{1}\,0]$
S1	$(1\,2\,3)\,[6\,3\,\bar{4}]$
S2	$(\bar{1}\,2\,3)\,[6\,\bar{3}\,4]$
S3	$(1\,\bar{2}\,3)\,[6\,\bar{3}\,\bar{4}]$
S4	$(\bar{1}\,\bar{2}\,3)\,[6\,3\,4]$
Brass1	$(1\,1\,0)\,[1\,\bar{1}\,2]$
Brass2	$(\bar{1}\,1\,0)\,[1\,1\,\bar{2}]$
Copper1	$(1\,1\,2)\,[1\,1\,\bar{1}]$

Copper2	$(\bar{1}\,1\,2)\,[1\,\bar{1}\,1]$

When loading orientations from an external file, '`file(`*`file_name`*`)`' assumes orientations described by Euler angles in Bunge convention (and active convention). To specify a different descriptor, use '`file(`*`file_name`*`,des=`*`descriptor`*`)`', where '*`descriptor`*' is among the descriptors listed above.

A.10 Crystal Symmetries

Crystal symmetries can be described using the following descriptors.

Key	**Descriptor**	**Number of operators**
`triclinic`	triclinic (Laue group $\bar{1}$)	24
`cubic`	cubic	24
`hexagonal`	hexagonal	1
`-1`	Laue group $\bar{1}$	1
`2/m`	Laue group $2/m$	2
`mmm`	Laue group mmm	4
`4/m`	Laue group $4/m$	4
`4/mmm`	Laue group $4/mmm$	8
`-3`	Laue group $\bar{3}$	3
`-3m`	Laue group $\bar{3}m$	6
`6/m`	Laue group $6/m$	6
`6/mmm`	Laue group $6/mmm$	12
`m-3`	Laue group $m\bar{3}$	12
`m-3m`	Laue group $m\bar{3}m$	24

Keys are available for ideal orientations (lowercased is accepted):

Cube	$(0\,0\,1)\,[1\,0\,0]$
Goss	$(0\,1\,1)\,[1\,0\,0]$
U	$(1\,0\,1)\,[\bar{1}\,0\,1]$
45NDCube	$(0\,0\,1)\,[1\,\bar{1}\,0]$
S1	$(1\,2\,3)\,[6\,3\,\bar{4}]$
S2	$(\bar{1}\,2\,3)\,[6\,\bar{3}\,4]$
S3	$(1\,\bar{2}\,3)\,[6\,\bar{3}\,\bar{4}]$
S4	$(\bar{1}\,\bar{2}\,3)\,[6\,3\,4]$
Brass1	$(1\,1\,0)\,[1\,\bar{1}\,2]$
Brass2	$(\bar{1}\,1\,0)\,[1\,1\,\bar{2}]$
Copper1	$(1\,1\,2)\,[1\,1\,\bar{1}]$
Copper2	$(\bar{1}\,1\,2)\,[1\,\bar{1}\,1]$

A.11 Colors and Color Maps

A.12 Colors

The available colors are provided below, with their corresponding RGB channel values. Any other color can be defined from the RGB channel values, under format '*`R_value|G_value|B_value`*'.

(0, 0, 0)	`black`	(255, 0, 0)	`red`
(0, 255, 0)	`green`	(0, 0, 255)	`blue`
(255, 255, 0)	`yellow`	(255, 0, 255)	`magenta`

(0, 255, 255)	cyan
(128, 0, 0)	maroon
(127, 255, 0)	chartreuse
(128, 128, 0)	olive
(0, 128, 128)	teal
(0, 191, 255)	deepskyblue
(64, 64, 64)	darkgray
(192, 192, 192)	silver
(139, 0, 0)	darkred
(255, 140, 0)	darkorange
(248, 248, 255)	ghostwhite
(0, 0, 205)	mediumblue
(245, 255, 250)	mintcream
(240, 128, 128)	lightcoral
(255, 127, 80)	coral
(255, 250, 240)	floralwhite
(255, 250, 205)	lemonchiffon
(0, 100, 0)	darkgreen
(240, 248, 255)	aliceblue
(255, 255, 224)	lightyellow
(0, 139, 139)	darkcyan
(70, 130, 180)	steelblue
(255, 245, 238)	seashell
(72, 61, 139)	darkslateblue
(255, 160, 122)	lightsalmon
(135, 206, 250)	lightskyblue
(240, 255, 240)	honeydew
(255, 218, 185)	peachpuff
(255, 99, 71)	tomato
(255, 105, 180)	hotpink
(255, 235, 205)	blanchedalmond
(255, 228, 181)	moccasin
(60, 179, 113)	mediumseagreen
(238, 130, 238)	violet
(255, 239, 213)	papayawhip
(188, 143, 143)	rosybrown
(139, 69, 19)	saddlebrown
(30, 144, 255)	dodgerblue
(222, 184, 135)	burlywood
(250, 240, 230)	linen
(64, 224, 208)	turquoise
(72, 209, 204)	mediumturquoise
(255, 228, 225)	mistyrose
(250, 235, 215)	antiquewhite
(50, 205, 50)	limegreen
(176, 196, 222)	lightsteelblue
(152, 251, 152)	palegreen
(245, 222, 179)	wheat
(230, 230, 250)	lavender
(144, 238, 144)	lightgreen
(47, 79, 79)	darkslategray
(46, 139, 87)	seagreen
(255, 255, 255)	white
(0, 0, 128)	navy
(0, 255, 127)	springgreen
(128, 0, 128)	purple
(128, 128, 128)	gray
(124, 252, 0)	lawngreen
(255, 69, 0)	orangered
(255, 250, 250)	snow
(0, 0, 139)	darkblue
(240, 255, 255)	azure
(255, 255, 240)	ivory
(255, 182, 193)	lightpink
(75, 0, 130)	indigo
(255, 192, 203)	pink
(250, 128, 114)	salmon
(127, 255, 212)	aquamarine
(255, 215, 0)	gold
(255, 165, 0)	orange
(224, 255, 255)	lightcyan
(139, 0, 139)	darkmagenta
(205, 133, 63)	peru
(255, 240, 245)	lavenderblush
(0, 250, 154)	mediumspringgreen
(184, 134, 11)	darkgoldenrod
(255, 228, 196)	bisque
(250, 250, 210)	lightgoldenrodyellow
(255, 248, 220)	cornsilk
(245, 245, 245)	whitesmoke
(112, 128, 144)	slategray
(253, 245, 230)	oldlace
(189, 183, 107)	darkkhaki
(0, 206, 209)	darkturquoise
(199, 21, 133)	mediumvioletred
(173, 255, 47)	greenyellow
(143, 188, 143)	darkseagreen
(255, 20, 147)	deeppink
(148, 0, 211)	darkviolet
(119, 136, 153)	lightslategray
(255, 222, 173)	navajowhite
(123, 104, 238)	mediumslateblue
(135, 206, 235)	skyblue
(245, 245, 220)	beige
(210, 180, 140)	tan
(216, 191, 216)	thistle
(233, 150, 122)	darksalmon
(65, 105, 225)	royalblue
(220, 20, 60)	crimson
(186, 85, 211)	mediumorchid
(240, 230, 140)	khaki
(175, 238, 238)	paleturquoise
(153, 50, 204)	darkorchid
(154, 205, 50)	yellowgreen

(138, 43, 226)	blueviolet
(107, 142, 35)	olivedrab
(244, 164, 96)	sandybrown
(102, 205, 170)	mediumaquamarine
(238, 232, 170)	palegoldenrod
(25, 25, 112)	midnightblue
(211, 211, 211)	lightgray
(100, 149, 237)	cornflowerblue
(178, 34, 34)	firebrick
(205, 92, 92)	indianred
(173, 216, 230)	lightblue
(165, 42, 42)	brown
(220, 220, 220)	gainsboro
(95, 158, 160)	cadetblue
(219, 112, 147)	palevioletred
(147, 112, 219)	mediumpurple
(85, 107, 47)	darkolivegreen
(106, 90, 205)	slateblue
(34, 139, 34)	forestgreen
(32, 178, 170)	lightseagreen
(218, 112, 214)	orchid
(160, 82, 45)	sienna
(176, 224, 230)	powderblue
(105, 105, 105)	dimgray
(210, 105, 30)	chocolate
(218, 165, 32)	goldenrod
(221, 160, 221)	plum

A.13 Color Maps

A.13.1 Color Map for Integer Values

The color map (also called *palette*) used to represent integer values is defined from the above color list, by excluding colors of brightness below 0.2 and above 0.8. The brightness is defined as the average of the channel values divided by 255. The resulting list of colors is: (1) red, (2) green, (3) blue, (4) yellow, (5) magenta, (6) cyan, (7) chartreuse, (8) springgreen, (9) olive, (10) purple, (11) teal, (12) gray, (13) deepskyblue, (14) lawngreen, (15) darkgray, (16) orangered, (17) silver, (18) darkorange, (19) mediumblue, (20) indigo, (21) lightcoral, (22) coral, (23) salmon, (24) aquamarine, (25) gold, (26) orange, (27) darkmagenta, (28) darkcyan, (29) peru, (30) steelblue, (31) mediumspringgreen, (32) darkslateblue, (33) darkgoldenrod, (34) lightsalmon, (35) lightskyblue, (36) tomato, (37) slategray, (38) hotpink, (39) darkkhaki, (40) darkturquoise, (41) mediumseagreen, (42) mediumvioletred, (43) violet, (44) greenyellow, (45) darkseagreen, (46) rosybrown, (47) deeppink, (48) saddlebrown, (49) darkviolet, (50) dodgerblue, (51) lightslategray, (52) burlywood, (53) mediumslateblue, (54) turquoise, (55) skyblue, (56) mediumturquoise, (57) tan, (58) limegreen, (59) darksalmon, (60) lightsteelblue, (61) royalblue, (62) palegreen, (63) crimson, (64) mediumorchid, (65) khaki, (66) lightgreen, (67) darkslategray, (68) darkorchid, (69) seagreen, (70) yellowgreen, (71) blueviolet, (72) palevioletred, (73) olivedrab, (74) mediumpurple, (75) sandybrown, (76) darkolivegreen, (77) mediumaquamarine, (78) slateblue, (79) forestgreen, (80) midnightblue, (81) lightseagreen, (82) orchid, (83) cornflowerblue, (84) sienna, (85) firebrick, (86) indianred, (87) dimgray, (88) chocolate, (89) brown, (90) goldenrod, (91) plum and (92) cadetblue.

A.13.2 Color Maps for Real Values

The color *map* used to represent real values is smooth and obtained by interpolation between nominal colors. Tinycolormap (https://github.com/yuki-koyama/tinycolormap) is used to generate standard color maps:

Python-style	**Matlab-style**	**GitHub-style**
magma	parula	github
inferno	heat	
plasma	hot	
viridis	jet	
cividis	gray	

and '`viridis`' is the default. See `https://github.com/yuki-koyama/tinycolormap` for illustrations.

Alternatively, any series of colors can be used to define a color map. Neper's legacy color map (version < 4) is '`blue,cyan,yellow,green`' and can be obtained using '`legacy`'.

Appendix B File and Directory Formats

B.1 Tessellation File (.tess)

Here are details on the `.tess` file format version `2.0`. Developers should note that read and write functions are available as '`neut_tess_fscanf`' and '`neut_tess_fprintf`', defined in directories `neut/neut_tess/neut_tess_fscanf` and `neut/neut_tess/neut_tess_fprintf`.

```
***tess
  **format
    format
  **general
    dim type
  **cell
    number_of_cells
 [*id
   cell1_id cell2_id ... ]
 [*seed
   seed_id seed_x seed_y seed_z seed_weight
    ... ]
 [*ori
   descriptor
    cellid_param1 cellid_param2 ...
    ... ]
 [*oridistrib
    cellid_distrib
    ... ]
 [*lam
    cell1_lam cell2_lam ... ]
 [*mode
    cell1_mode cell2_mode ... ]
 [*crysym
    crysym]
  **vertex
    total_number_of_vertices
    ver_id  ver_x ver_y ver_z ver_state
    ...
  **edge
    total_number_of_edges
    edge_id ver_1 ver_2 edge_state
    ...
  **face
    total_number_of_faces
    face_id number_of_vertices ver_1   ver_2   ...
           number_of_edges    edge_1* edge_2* ...
           face_eq_d face_eq_a face_eq_b face_eq_c
           face_state face_point
    face_point_x face_point_y face_point_z
    ...
  **polyhedron
    total_number_of_polyhedra
```

```
    poly_id number_of_faces face_1* face_2* ...
    ...
  **domain
   *general
    dom_type
   *vertex
    total_number_of_dom_vertices
    dom_ver_id  dom_ver_x dom_ver_y dom_ver_z dom_ver_label
                number_of_dom_tess_vertices ver_1
    ...
   *edge
    total_number_of_dom_edges
    dom_edge_id number_of_dom_vertices [dom_ver_1 dom_ver_2]
                dom_edge_label
                number_of_dom_tess_edges edge_1
      edge_2 ...
    ...
   *face
    total_number_of_dom_faces
    dom_face_id number_of_dom_vertices dom_ver_1  dom_ver_2  ...
                number_of_dom_edges    dom_edge_1 dom_edge_2
             ...
                dom_face_type
                number_of_params dom_face_param1 dom_face_param2 ...
                dom_face_label
                number_of_dom_tess_faces
dom_tess_face_1 dom_tess_face_2 ...
   ...
  **periodic
   *general
    per_x per_y per_z
    per_dist_x per_dist_y per_dist_z
   *seed
    secondary_seed_qty
    secondary_seed_id primary_seed_id per_shift_x per_shift_y per_shift_z
   ...
   *vertex
    secondary_ver_qty
    secondary_ver_id primary_ver_id per_shift_x per_shift_y per_shift_z
   ...
   *edge
    secondary_edge_qty
    secondary_edge_id primary_edge_id per_shift_x per_shift_y per_shift_z
                                                              secondary_edge_ori
   ...
   *face
    secondary_face_qty
    secondary_face_id primary_face_id per_shift_x per_shift_y per_shift_z
                                                              secondary_face_ori
   ...
  **scale
   *general
```

```
 number_of_scales
*cellid
 cell1_id cell1_scale1 cell1_scale2 ... cell1_scalenumber_of_scales
...
***end
```

where (with identifiers being integer numbers),

- `***tess` denotes the beginning of a tessellation file.
- `**format` denotes the beginning of the format field.
- *`format`* is the file format, currently '`2.0`' (character string).
- `**general` denotes the beginning of the general information field.
- *`dim`* is the dimension of the tessellation (1, 2 or 3).
- *`type`* is the type of tessellation (always '`standard`').
- `**cell` denotes the beginning of the cell field.
- *`number_of_cells`* is the number of cells.
- `*id` denotes the beginning of an optional identifier field. It the field is not present, the cells are considered to be numbered contiguously from 1.
- *`cell1_id`*, *`cell2_id`*, ... are the actual identifiers of the cells.
- `*lam` denotes the beginning of an optional lamella identifier field.
- *`cell1_lam`*, *`cell2_lam`*, ... are the lamella identifiers of the cells.
- `*mode` denotes the beginning of an optional mode identifier field.
- *`cell1_mode`*, *`cell2_mode`*, ... are the mode identifiers of the cells.
- *`crysym`* is the crystal symmetry (`triclinic`, `cubic` or `hexagonal`).
- `*seed` denotes the beginning of a seed field.
- *`seed_id`* is the identifier of a seed and ranges from `1` to *`number_of_cells`*.
- *`seed_x`*, *`seed_y`* and *`seed_z`* are the three coordinates of a seed (real numbers).
- *`seed_weight`* is the weight of a seed (real number).
- `*ori` denotes the beginning of an optional crystal orientation field.
- `descriptor` is the descriptor used to parametrize the crystal orientations. See Section A.9 [Rotations and Orientations], page 75, for the list of available descriptors.
- *`cellid_param1`*, *`cellid_param2`*, ... are the values of the orientation descriptor of cell *id*.
- `*oridistrib` denotes the beginning of an optional crystal orientation distribution field.
- *`cellid_distrib`* is the value of the orientation distribution of cell *id*.
- `**vertex` denotes the beginning of the vertex field.
- *`total_number_of_vertices`* is the total number of vertices.
- *`ver_id`* is the identifier of a vertex and ranges from `1` to `total_number_of_vertices`.
- *`ver_x`*, *`ver_y`* and `ver_z` are the three coordinates of a vertex (real numbers).
- *`ver_state`* is an integer indicating the state of a vertex. For a standard tessellation (no regularization), it equals `0`. For a regularized tessellation, it equals `0` if the vertex has not been modified by regularization and is higher than `0` otherwise.
- `**edge` denotes the beginning of the edge field.
- *`total_number_of_edges`* is the total number of edges.
- *`edge_id`* is the identifier of an edge and ranges from `1` to `total_number_of_edges`.
- *`ver_1`*, *`ver_2`*, `...` are identifiers of vertices.

- *edge_state* is an integer indicating the state of an edge (always 0).
- **face denotes the beginning of the face field. It is present for a tessellation of dimension 2 or 3.
- *total_number_of_faces* is the total number of faces.
- *face_id* is the identifier of a face and ranges from 1 to total_number_of_faces.
- *number_of_vertices* is the number of vertices of a face.
- *number_of_edges* is the number of edges of a face.
- *edge_1**, *edge_2**, ... are identifiers of the edges of a face, signed according to their orientation in the face.
- *face_eq_a*, *face_eq_b*, *face_eq_c* and *face_eq_d* are the parameters of the equation of a face: $face\_eq\_a\,x + face\_eq\_b\,y + face\_eq\_c\,z = face\_eq\_d$. The parameters are scaled so that $face\_eq\_a^2 + face\_eq\_b^2 + face\_eq\_c^2 = 1$.
- *face_state* is an integer indicating the state of a face. For a standard tessellation (no regularization), it equals 0. For a regularized tessellation, it equals 0 if it has not been modified by regularization and 1 otherwise.
- *face_point* is an integer indicating the point used for the interpolation of a face. For a standard tessellation (no regularization), it equals 0. For a regularized tessellation: if the point is the face barycentre, it equals 0; if the point is one of the face vertices, it equals to the position of the vertex in the list of vertices of the face. It equals -1 if the point is undefined.
- *face_point_x*, *face_point_y* and *face_point_z* are the coordinates of the point used for the interpolation of a face (equal 0 if undefined).
- **polyhedron denotes the beginning of the polyhedron field. It is present for a tessellation of dimension 3.
- *total_number_of_polyhedra* is the total number of polyhedra.
- *poly_id* is the identifier of a polyhedron and ranges from 1 to total_number_of_polyhedra.
- *number_of_faces* is the number of faces of a polyhedron.
- *face_1**, *face_2**, ... are identifiers of the faces of a polyhedron, signed according to their orientations in the polyhedron (positive if the normal of the face is pointing outwards and negative if it is pointing inwards).
- **domain denotes the beginning of the domain field.
- *general denotes the beginning of the domain general information field.
- *dom_type* is the type of the domain (one of cube, cylinder, square, circle, poly and planes).
- *vertex denotes the beginning of the domain vertex field.
- *total_number_of_dom_vertices* is the total number of domain vertices.
- *dom_ver_id* is the identifier of a domain vertex and ranges between 1 to total_number_of_dom_vertices.
- *dom_ver_x*, *dom_ver_y* and dom_ver_z are the three coordinates of a domain vertex (real numbers).
- *dom_ver_label* is the label of a domain vertex.
- *number_of_dom_tess_vertices* is the number of tessellation vertices of a domain vertex (must be 1).
- *edge denotes the beginning of the domain edge field (for a tessellation of dimension 2 or 3).

- *total_number_of_dom_edges* is the total number of domain edges.
- *dom_edge_id* is the identifier of a domain edge and ranges between 1 to total_number_of_dom_edges.
- *number_of_dom_vertices* is the number of domain vertices of a domain edge or a domain face.
- *dom_ver_1*, *dom_ver_2*, ... are identifiers of the domain vertices of a domain edge or face.
- *dom_edge_label* is the label of a domain edge.
- *number_of_dom_tess_edges* is the number of tessellation edges of a domain edge.
- *face denotes the beginning of the domain face field (for a tessellation of dimension 3).
- *total_number_of_dom_faces* is the total number of domain faces.
- *dom_face_id* is the identifier of a domain face and ranges from 1 to total_number_of_dom_faces.
- *number_of_dom_edges* is the number of domain edges of a domain face.
- *dom_edge_1*, *dom_edge_2*, ... are identifiers of the domain edges of a domain face.
- *dom_face_type* is the type of a face, among 'plane', 'cylinder' or 'sphere'.
- *number_of_params* is the number of parameters of a domain face.
- *dom_face_param1*, *dom_face_param2*, ... are the parameters of a domain face. For a planar face, they are the parameters of the equation of the face, listed in the order *face_eq_d*, *face_eq_a*, face_eq_b and *face_eq_c*. For a cylindrical face, they are the coordinates of the base point, the axis and the radius. For a spherical face, they are the coordinates of the centre and the radius.
- *dom_face_label* is the label of a domain face. If *dom_type* is 'cube', it is one of 'x0', 'x1', 'y0', 'y1', 'z0' or 'z1'. If *dom_type* is 'cylinder', it is one of 'z0', 'z1', 'f1', 'f2', ... Otherwise, it is one of 'f1', 'f2', ...
- *number_of_dom_tess_faces* is the number of tessellation faces of a domain face.
- *dom_tess_face_1*, *dom_tess_face_2*, ... are the identifiers of the tessellation faces of a domain face.
- ***end denotes the end of a tessellation file.
- **periodicity denotes the beginning of the periodicity field.
- *general denotes the beginning of the periodicity general information field.
- *per_x*, *per_y* and *per_z* are booleans indicating x, y, and z periodicity.
- *per_dist_x*, *per_dist_y* and *per_dist_z* are the periodicity distances along x, y, and z.
- *seed denotes the beginning of the periodicity seed field.
- *secondary_seed_qty* is the number of secondary seeds.
- *secondary_seed_id* is the identifier of a secondary seed.
- *primary_seed_id* is the identifier of the primary of a secondary seed.
- *per_shift_x*, *per_shift_y* and *per_shift_z* are the shifts of a secondary seed (or vertex, etc.) relative to its primary, along x, y and z. The values can be -1, 0 or 1.
- *vertex denotes the beginning of the periodicity vertex field.
- *secondary_vertex_qty* is the number of secondary vertices.
- *secondary_vertex_id* is the identifier of a secondary vertex.
- *primary_vertex_id* is the identifier of the primary of a secondary vertex.
- *edge denotes the beginning of the periodicity edge field.
- *secondary_edge_qty* is the number of secondary edges.
- *secondary_edge_id* is the identifier of a secondary edge.

- *primary_edge_id* is the identifier of the primary of a secondary edge.
- *secondary_edge_ori* is the orientation of the secondary edge with respect to the primary edge: 1 if identical, -1 if opposite.
- *face denotes the beginning of the periodicity face field (for a tessellation of dimension 3).
- *secondary_face_qty* is the number of secondary faces.
- *secondary_face_id* is the identifier of a secondary face.
- *primary_face_id* is the identifier of the primary of a secondary face.
- *secondary_face_ori* is the orientation of the secondary face with respect to the primary face: 1 if identical, -1 if opposite.
- *number_of_scales* is the number of scales.
- *cell1_scale1*, *cell1_scale2*, ... are the identifiers of the cells of the scale-1, scale-2, ... tessellations which the cell belongs to.

B.2 Raster Tessellation File (.tesr)

Here are details on the .tesr file format version 2.0. Developers should note that read and write functions are available as 'neut_tesr_fscanf' and 'neut_tesr_fprintf', defined in directories neut/neut_tesr/neut_tesr_fscanf and neut/neut_tesr/neut_tesr_fprintf. Compared to a tessellation file (.tess), a raster tessellation file can include cell morphological properties such as their centroids or volumes. This is motivated by the fact that, for a raster tessellation, these properties are both in small number and relatively expensive to compute, and so are stored once known. Square brackets ([ ]) denote optional fields.

```
***tesr
  **format
    format data_format
  **general
    dimension
    size_x size_y [size_z]
    voxsize_x voxsize_y [voxsize_z]
 [*origin
    origin_x origin_y [origin_z]]
 [*hasvoid has_void]
[**cell
    number_of_cells
 [*id
    cell1_id cell2_id ...]
 [*seed
   seed_id seed_x seed_y [seed_z] seed_weight
    ...]
 [*ori
   descriptor
    cell1_param1 cell1_param2 ...
    cell2_param1 cell2_param2 ...
   ...]
 [*coo
    cell1_x cell1_y [cell1_z]
    cell2_x cell2_y [cell2_z]
    ...]
 [*vol
    cell1_vol
```

```
    cell2_vol
    ...]
 [*convexity
    cell1_convexity
    cell2_convexity
    ...]
]
[*crysym
   crysym
]
  **data
    vox1_cell vox2_cell ...
 or
  *file data_file_name
[**oridata
   descriptor
   vox1_param1 vox1_param2 ...
   vox2_param1 vox2_param2 ...
 or
   descriptor
  *file oridata_file_name
]

***end
```

where

- `***tesr` denotes the beginning of a raster tessellation file.
- `**format` denotes the beginning of the format field.
- *`format`* is the file format, currently '`2.0`' (character string).
- *`data_format`* is the format of the data in field `**data`. It can be either `ascii`, `binary8` (8-bit binary), `binary16` (16-bit binary, LittleEndian), `binary16_big` (16-bit binary, BigEndian), `binary32` (32-bit binary, LittleEndian) or `binary32_big` (32-bit binary, BigEndian).
- `**general` denotes the beginning of the general information field.
- *`dimension`* is the dimension of the raster tessellation.
- *`size_x`*, *`size_y`* and *`size_z`* are the raster sizes along the coordinate axes. The number of sizes must match *dimension*.
- *`voxsize_x`*, *`voxsize_y`* and *`voxsize_z`* are the voxel (pixel, in 2D) sizes along the coordinate axes. The number of sizes must match *dimension*.
- `*origin` denotes the beginning of an optional origin field.
- *`origin_x`*, *`origin_y`* and *`origin_z`* are the (absolute) coordinates of the origin of the raster tessellation along the coordinate axes. The number of coordinates must match *dimension*.
- `*hasvoid` denotes the beginning of an optional has-void field.
- *`has_void`* is a boolean indicating whether the tessellation contains void voxels (which have a cell id of 0).
- `**cell` denotes the beginning of an optional cell field.
- *`number_of_cells`* is the number of cells.
- `*id` denotes the beginning of an optional identifier field. If the field is present, the cell identifiers listed under `**data` are supposed to be numbered contiguously from 1 (or 0 in

case of void), and their actual identifiers are considered to be the ones provided in the list. The actual identifiers are used in output files.

- *cell1_id*, *cell2_id*, ... are the actual identifiers of the cells.
- `*seed` denotes the beginning of a seed field.
- *seed_id* is the identifier of a seed and ranges from `1` to `number_of_cells`.
- *seed_x*, *seed_y* and `seed_z` are the three coordinates of a seed (real numbers).
- *seed_weight* is the weight of a seed (real number).
- `*ori` denotes the beginning of an optional crystal orientation field.
- `descriptor` is the descriptor used to parametrize the crystal orientations. See Section A.9 [Rotations and Orientations], page 75, for the list of available descriptors.
- *cellid_param1*, *cellid_param2*, ... are the values of the orientation descriptor of cell *id*.
- `*coo` denotes the beginning of an optional centroid field.
- *cellid_x*, *cellid_y* and *cellid_z* are the coordinates of the centroids of cell *id*.
- `*vol` denotes the beginning of an optional volume field.
- *cellid_vol* is the volume of cell *id*.
- `*convexity` denotes the beginning of an optional convexity field.
- *cellid_convexity* is the convexity of cell *id*.
- `*crysym` denotes the beginning of an optional crystal symmetry field.
- *crysym* is the crystal symmetry (`triclinic`, `cubic` or `hexagonal`).
- `**data` denotes the beginning of the data field. Data can be provided in the `.tesr` file or in a separate file, using `*file`, see below.
- *voxid_cell* is the cell voxel *id* belongs to. Voxels must be listed in column-major order (x varying first, y varying second and z varying last). The cell identifiers should start from 1. Use 0 for voids.
- `*file` denotes the beginning of a file field.
- `data_file_name` is the name of a file that contains the data. It must be located in the same directory as the parent tesr file, or its path relative to the parent tesr file must be provided. Typically, it is a `.raw` file.
- `**oridata` denotes the beginning of the orientation data field. Data can be provided in the `.tesr` file or in a separate file, using `*file`, see below.
- *voxid_param1*, *voxid_param2*, ... are the values of the orientation descriptor of voxel *id*. Orientations must be listed in column-major order (x varying first, y varying second and z varying last). Arbitrary orientations can be used for void voxels (*voxid_cell* = `0`). These data must be written under format *data_format*, in terms of ASCII or binary. In the case of binary format, double-precision numbers are considered.
- `oridata_file_name` is the name of a file that contains the orientation data. It must be located in the same directory as the parent tesr file, or its path relative to the parent tesr file must be provided. Typically, it is a `.raw` file.

B.3 Multiscale Cell File

A multiscale cell file provides cell-by-cell values for a multiscale tessellation and can be loaded using '`msfile(`*filename*`)`'[1]. The file contains, for each cell, its *multiscale identifier*, *mid*, and the value(s). A *cell multiscale identifier* (*mid*) is a character string identifying a cell at a specific scale. For a given cell, C, *mid* combines the identifiers of the cells that C belongs to, at successive

[1] As of version 3.5.0, '`msfile(`*filename*`)`' should be preferred over '`file(`*filename*`)`'

scales, to its own `id`, separated by '`::`'. For a 1-scale tessellation, *mid* equals *id*. For a 2-scale tessellation composed of 2×3 cells, the *mid*s are equal to `1::1`, `1::2`, `1::3`, `2::1`, `2::2` and `2::3`. The domain (which can be considered as a cell at scale 0), *mid* is nil. An example of a multiscale cell file that could be used to define the numbers of cells of a 3-scale tessellation is:

```
2
1 2
2 4
1::1 3
1::2 4
2::1 5
2::2 6
2::3 7
2::4 8
```

The file could be used in `-T` as: `-n msfile(`*`filename`*`)::msfile(`*`filename`*`)::msfile(`*`filename`*`)`. The first instance of '`msfile(`*`filename`*`)`' reads the number of scale-1 cells in line 1, the second instance of '`msfile(`*`filename`*`)`' reads the number of scale-2 cells in lines 2–3, and the third instance of '`msfile(`*`filename`*`)`' reads the number of scale-3 cells in lines 4–7.

B.4 Position File

A position file lists the coordinates of a given number of points. The file must contain 1 coordinate per point in 1D, 2 coordinates per point in 2D and 3 coordinates per point in 3D. While the dimension can be known from the context in which the file is read, it can also be specified by appending '`:`*`dim`*' to the name of the position file, where *dim* is the dimension. A coordinate can be an integer or real number. A real number can have an arbitrary number of digits, but the decimal mark must be '`.`'. The coordinates can be separated from each other by spaces, tabulators or newlines (any number as well as arbitrary combinations of them are supported). However, a good practice is to format the file with one line per point. An example of a position file containing 5 points in 3D is:

```
2.1235 9.4544 5.2145
5.9564 3.6884 9.2145
2.2547 3.2658 8.2514
8.2515 9.4157 2.9454
0.5874 4.2848 2.4874
```

B.5 Mesh File (`.msh`)

Here are details on the native `.msh` (adapted from Gmsh's msh format version `2.2`). Developers should note that read and write functions are available as '`neut_msh_fscanf`' and '`neut_msh_fprintf`', defined in directories `neut/neut_msh/neut_msh_fscanf` and `neut/neut_msh/neut_msh_fprintf`.

```
$MeshFormat
2.2 file_type data_size
$EndMeshFormat
$Nodes
number_of_nodes
node_id node_x node_y node_z
...
$EndNodes
$Elements
number_of_elements
```

```
elt_id elt_type number_of_tags tag1 ... elt_id_node1 ...
...
$EndElements
$Periodicity
number_of_periodicities
secondary_node_id primary_node_id per_vect_x per_vect_y per_vect_z
...
$EndPeriodicity
$NSets
number_of_nsets
nset1_label
nset_node_nb
nset_node1
nset_node2
...
nset2_label
...
$EndNSets
$Fasets
number_of_fasets
faset1_label
faset_elt_nb
faset_elt_id faset_elt_id_node1 ...
...
faset2_label
...
$EndFasets
$NodePartitions
number_of_nodes
node_id node_partition
...
$EndNodePartitions
$PhysicalNames
number_of_physical_names
physical_dimension physical_id physical_name
...
$EndPhysicalNames
$ElsetOrientations
number_of_elsets orientation_descriptor
elset_id ori_des1 ...
...
$EndOrientations
$ElementOrientations
number_of_elements orientation_descriptor
element_id ori_des1 ...
...
$EndElementOrientations
$Groups
group_entity
number_of_group_entities
entity_id group
...
```

```
$EndGroups
```

where

- `$MeshFormat` denotes the beginning of a mesh format field.
- *`file_type`* is equal to `0` for an ASCII file and `1` for a binary file.
- *`data_size`* is an integer equal to the size of the floating point numbers used in the file (= `sizeof (double)`).
- `$EndMeshFormat` denotes the end of a mesh format field.
- `$Nodes` denotes the beginning of a node field.
- *`number_of_nodes`* is the number of nodes.
- *`node_id`* is the identifier of a node and ranges from `1` to *`number_of_nodes`*.
- *`node_x`*, *`node_y`* and *`node_z`* are the three coordinates of a node (real numbers).
- `$EndNodes` denotes the end of a node field.
- `$Elements` denotes the beginning of an element field.
- *`number_of_elements`* is the number of elements.
- *`elt_type`* is an integer specifying the type of elements: `15` for a 0D element, `1` for a 1st-order 1D element (2 nodes), `8` for a 2nd-order 1D element (3 nodes), `2` for a 1st-order triangular element (3 nodes), `3` for a 1st-order quadrangular element (4 nodes), `9` for a 2nd-order triangular element (6 nodes), `16` for a 2nd-order quadrangular element (8 nodes), `10` for a 2nd-order quadrangular element (9 nodes), `4` for a 1st-order tetrahedral element (4 nodes), `5` for a 1st-order hexahedral element (4 nodes), `11` for a 2nd-order tetrahedral element (10 nodes), `6` for a 1st-order prismatic element (6 nodes), `18` for a 2nd-order prismatic element (15 nodes).
- *`number_of_tags`* is the number of tags, and *`tag1 ...`* are the tags. In the general case, the number of tags is equal to 3, the first and second tags are the elset and the third tag is the element partition. The mesh partition is non-zero only for the higher-dimension elements of a mesh which was previously partitioned.
- *`elt_id_node1 ...`* are the nodes associated to an element. The number of nodes depends on the element type ('*`elt_type`*').
- `$EndElements` denotes the end of an element field.
- `$Periodicity` denotes the beginning of a periodicity field.
- *`number_of_periodicities`* is the number of periodicities.
- *`primary_node_id`* is the identifier of the primary node.
- *`secondary_node_id`* is the identifier of the secondary node.
- *`per_vect_x per_vect_y per_vect_z`* are the scaled components of the vector going from the primary node to the secondary node (-1, 0 or 1).
- `$EndPeriodicity` denotes the end of a periodicity field.
- `$NSets` denotes the beginning of an nset field.
- *`number_of_nsets`* is the number of nsets.
- *`nset1_label`*, *`nset2_label ...`* are the labels of the nsets.
- *`nset_node_nb`* is the number of nodes of an nset.
- *`nset_node_id1`*, *`nset_node_id1 ...`* are the identifiers of the nodes of an nset.
- `$EndNSets` denotes the end of an nset field.
- `$Fasets` denotes the beginning of a faset field.
- *`number_of_fasets`* is the number of fasets.
- *`faset1_label`*, *`faset2_label ...`* are the labels of the fasets.

- *faset_elt_nb* is the number of elements of a faset.
- *faset_elt_id ...* are the identifiers of the elements of a faset (3D elements adjacent to the boundary).
- *faset_elt_id_node1 ...* are the nodes of an element of a faset.
- `$EndFasets` denotes the end of a faset field.
- `$NodePartitions` denotes the beginning of a node partition field.
- *nodeid_partition* is the partition of node *id* (ranging from 1 to the total number of partitions).
- `$EndNodePartitions` denotes the end of a node partition field.
- `$PhysicalNames` denotes the beginning of a physical name field.
- *number_of_physical_names* is the number of physical names. There are as many names as physical entities, and the physical entities correspond to all tessellation vertices, edges, faces and polyhedra (i.e., mesh 0D, 1D, 2D and 3D elsets).
- *physical_dimension* is the dimension of a physical entity and can be equal to 0, 1, 2 or 3.
- *physical_id* is the id of a physical entity. It ranges from 1 to the number of 0D elsets (tessellation vertices) for the 0D entities, 1 to the number of 1D elsets (tessellation edges) for the 1D entities, 1 to the number of 2D elsets (tessellation faces) for the 2D entities and 1 to the number of 3D elsets (tessellation polyhedra) for the 3D entities.
- *physical_name* is the name of a physical entity, under the form '`ver`*id*' for 0D elsets (tessellation vertices), '`edge`*id*' for 1D elsets (tessellation edges), '`face`*id*' for 2D elsets (tessellation faces) and '`poly`*id*' for 3D elsets (tessellation polyhedra), where '*id*' ranges from 1 to the number of elsets.
- `$EndPhysicalNames` denotes the end of a physical name field.
- `$ElsetOrientations` denotes the beginning of an elset orientation field.
- *number_of_elsets* is the number of elsets.
- *orientation_descriptor* is the orientation descriptor.
- *elset_id* is the elset id.
- *ori_des1 ...* is the orientation, following '*orientation_descriptor*'.
- `$EndElsetOrientations` denotes the end of an elset orientation field.
- `$ElementOrientations` denotes the beginning of an element orientation field.
- *number_of_elements* is the number of elements.
- *element_id* is the element id.
- `$EndElementOrientations` denotes the end of an element orientation field.
- `$Groups` denotes the beginning of a group field.
- *group_entity* is the entity for which groups are defined, which must be '`elset`'.
- *number_of_group_entities* is the number of group entities (number of elsets).
- *entity_id* is the id of an entity.
- *group* is the group of the entity.
- `$EndGroups` denotes the end of a group field.

B.6 Simulation Directory (`.sim`)

Here are details on the `.sim` simulation directory (the `.sim` extension is entirely optional). The directory is structured as follows:

```
simulation.sim
```

```
|-- report
|-- inputs
| |-- job.sh
| |-- simulation.config
| |-- simulation.msh
| `-- simulation.tess
`-- results
    |-- elements
    |   |-- ori
    |   | |-- ori.step0
    |   | |-- ori.step1
    |   |   `-- ...
    |   `-- ...
    `-- nodes
        |-- coo
        | |-- coo.step0
        | |-- coo.step1
        |   `-- ...
        `-- ...
```

where

- `report` is a report file containing information on the simulation and the content of the simulation directory. This file is mainly for internal use.
- `inputs` is an input file directory containing the tessellation file (`.tess`, if found in the input directory), the mesh file (`.msh`), the FEPX configuration file (`.config`), and all script files (`*.sh`, likely including a job submission file).
- `results` is the result directory.
- `results/nodes` is the node result directory.
- `results/elements` is the element result directory.
- `results/nodes` or `elements/`*`res`* is the directory for result '*`res`*'. The directory contains one file per simulation step, named *`res`*`.step`*`nb`*, where '*`nb`*' is the step number, ranging from 0 (for the initial state) to the total number of steps.

Results can have integer values, real values, vectorial values or tensorial values. In the result files, values for the different entities (nodes, elements, etc.) are written on successive lines, with components written on successive columns (space delimited). The components of a vector, *`v`*, are written as *`v1 v2 v3`*. The components of a symmetrical tensor, *`t`*, are written using Voigt notation, as *`t11 t22 t33 t23 t31 t12`*. The components of a skwe-symmetrical tensor, *`t`*, are written using *`t12 t13 t23`*. The components of a non-symmetrical tensor, *`t`*, are written as *`t11 t12 t13 t21 t22 t23 t31 t32 t33`*.

Appendix C Developer's Guide

This chapter provides information for anyone who plans to contribute to Neper or wishes to better understand how it works. The code structure is detailed and information are given on how to efficiently contribute to it. If you are missing information, complain!

C.1 Code Structure

The Neper root directory content is as follows (the slash character '`/`' is employed to denote directories),

- `COPYING`: license terms;
- `README.md`: generation information on Neper;
- `VERSIONS`: information on the versions of Neper;
- `src/`: source code directory;
- `doc/`: documentation directory;
- `utils/`: utilities directory.

Details on the '`src/`' and '`doc/`' directories are provided in the following.

C.1.1 Source Code

Neper's source code is located in directory `src/` and roughly consists of 150,000 lines shared between 320 directories and 1200 text files. The '`src/`' directory contains the following files and directories,

- `neper_.h` and `neper.c`

  These are the main source code header file and source code file of Neper. '`neper.c`' contains Neper's '`main`' function. It reads the arguments passed at the command line and runs the corresponding functions, which can be one of the program module.

- `neper_t/`, `neper_m/`, `neper_s/` and `neper_v/`

  These are directories that contain the source code of each of the program modules. The modules aim to be independent from each other; that is, a function of one module will never calls a function of another module (with a few exceptions).

- `neut/`

  '`neut`' stands for *Neper utilities*. The directory contains utility functions specific to Neper and used by several modules.

- `contrib`

  This directory contains utility functions not specific to Neper. The first one is '`ut`', which is a collection of general-purpose, low-level C functions (memory allocation, etc.). The second one is '`orilib`', which is a collection of routines for orientation manipulation (see `http://orilib.sourceforge.net`). The third one is nanoflann, a library for nearest neighbor searching (see `https://github.com/jlblancoc/nanoflann`), the fourth one is openGJK, a library for fast point-simplex distance computations (`https://github.com/MattiaMontanari/openGJK`), the firsth one is muparser, a library for interprating mathematical and logical expressions (see `http://beltoforion.de/article.php?a=muparser`), and the last one is tinycolormap, a library for color maps (`https://github.com/yuki-koyama/tinycolormap`). Although these libraries are also distributed alone (and might be already installed on your system), they are included into Neper instead of being considered as dependencies (contrary to the GSL, for example) to facilitate installation.

- `CMakeLists.txt`, `neper_config.h.in` and `cmake`

  These files and directories are specific to the building system, CMake. `CMakeLists.txt` is the CMake source file, which tells CMake where to find the program source files, how to

manage dependencies, where to install Neper, etc. `neper_config.h.in` is a small configuration file that is useful to CMake for managing dependencies and program version numbers. `cmake` contains `.cmake` files which help CMake locating the dependencies on the system (library and header files).

A module directory, `neper_X`, where '*X*' stands for the module letter (one of '`t`', '`m`', '`s`' or '`v`'), is structured as follows,

- `neper_X.h`, `neper_X_.h` and `neper_X.c`

  These are the source code header files and source code file of the module. `neper_X.c` contains the module function, '`neper_X`'. `neper_X_.h` is the source code header file, which is `#include`'ed in `neper_X.c` and contains a bunch of `#include`s to all necessary library header files. `neper_X.h` contains the prototype of the module function and is `#include`'ed in `neper_.h`. Hence, files `_.h` are local header files while files `.h` are header files `#include`'ed into an upper-level source code header file. This is true everywhere in the source code. Moreover, any function specific to module *X* is prefixed '`neX_`'.
- `neX_input` and `structIn_X.h`

  The '`neX_input`' directory contains functions for reading the value of the arguments passed to module *X* from the command line. The information are recorded into an '`IN_X`' C structure, which is declared in file '`structIn_X.h`'.
- `neX_foo`, `neX_bar`, etc.

  Each of these directories is associated to a specific task of the module and contains a function of the same name ('`neX_foo`', etc.) which is called from function '`neper_X`'. Each directory contains a directory tree structure.
- `CMakeLists.txt`

  This file tells CMake where to find the source files and how to manage dependencies in the module. It is used by the upper-level `CMakeLists.txt` file (there is no lower-level `CMakeLists.txt` file).

The `neut` directory is roughly structured as follows,

- `CMakeLists.txt`

  This file tells CMake where to find the source files and how to manage dependencies in the module. It is used by the upper-level `CMakeLists.txt` file (there is no lower-level `CMakeLists.txt` file).
- `neut.h` and `neut_X.h`

  These files are source code header files that `#include` header files of `neut` (which contain function prototypes) and are `#include`d in the modules. `neut.h` `#include`s all header files while the three others `#include` header files only necessary to the corresponding module (this speeds up compilation at development stage).
- `neut_structs`

  This directory contains header files which defines all C structures used in the program.
- `neut_foo`, `neut_bar`, etc.

  Each of these directories contain functions specific to a particular C structure. For example, `neut_tess` contains functions relative to the '`TESS`' structure, which describes a tessellation.

C.1.2 Documentation

Neper's documentation is located in directory `doc`. It is written in Texinfo, the GNU software documentation system. The documentation consists of a collection of `.texi` files (text files). The documentation may be compiled in PDF, info or html format by running `make pdf`, `make info` or `make html`, respectively. In official releases, both the PDF and info documentation files are built and included in the archive.

C.2 Contributing to Neper

The Neper development repository is hosted on GitHub: `https://github.com/rquey/neper`. Code contributions to be included in Neper's official (public) version should be submitted as pull requests on this repository.

C.2.1 Coding Conventions

Neper is written following the GNU Coding Standards (`http://www.gnu.org/prep/standards`), with the exception that braces are not indented (because there is so often 3+ loop levels in Neper). Please follow this convention. Here are a few tips and other remarks,

- For Vim, put the following commands in file `$HOME/.vimrc`:

```
:set sw=2
:set cindent
:syntax enable
:set textwidth=72
```

- You can run `indent -bli0` *`source_files`* for automatic formatting.
- Break up the code into meaningful chunks using blank lines. Always use a single blank line to separate parts of the code.
- Neper admits no compilation warnings. Please fix up all of them.
- Please help us maintaining good documentation by documenting any capability you may add.

C.2.2 Adding a New Option

In modules -T and -M, adding a new option can be done by following these steps:

- Add a variable to the '`IN_X`' structure to record the value of the option (file `structIn_X.h`).
- If necessary, allocate / free the variable in the `neX_in_set_zero` and `neX_in_free` functions (file `neX_input1.c`) Assign it a default value in `net_input_options_default` (file `neX_input3.c`).
- Add the option to the option list in `net_input_options_set` (file `neX_input3.c`), taking as an example another option of the same type (integer, etc.).
- Where appropriate in the source code, add a new function for the new option (if necessary in a new file or directory). The function should be executed depending on the value of the option.
- If adding one or several files or directories, add the source file(s) to the source file list in the `CMakeLists.txt` file of the corresponding module.
- Make sure the whole thing compiles and runs properly for your purpose.
- Make sure your own changes did not break anything in the rest of the code by running full testing, using `make test` (or `ctest`). You may also want to add a test specific to the new option.

In module -V, options are processed differently. Instead of being recorded in a C structure, they are read one after the other and associated functions are executed along the way. To add a new option, take an existing option as an example.

C.2.3 Compilation Options

For development, several compilation options can be changed from their default values. This must be done at configuration stage, using commands '`ccmake ..`' or '`cmake-gui ..`'. The compilation options are

- `DEVEL_DEBUGGING_FLAG`

  Setting the option to `ON` turns on the debugging compilation flag '`-g`', which is required for debugging with `gdb` and `valgrind`, and turns on the compilation flag '`-Werror`', which makes all compilation warnings into errors.
- `DEVEL_DEBUGGING_TEST`

  Setting the option to `ON` runs internal tests during Neper execution at places where the code is otherwise considered robust.
- `DEVEL_OPTIMIZATION`

  Setting this option to `OFF` disables code optimization, which is useful for debugging with `gdb` and `valgrind`.
- `DEVEL_PROFILING`

  Setting this option to `ON` turns on the code profiling compilation flag '`-pg`', which is required for profiling with `gprof`. This is a highy CPU-sensitive option, which should be used only when profiling is actually carried out.

C.2.4 Making a Commit

A `neper-commit` script is available in the `utils` directory. Running this script creates a Git commit (just as `git commit`) and handles the additional tasks of updating Neper's version number wherever needed in the code and documentation, and opening the `VERSIONS` file for you to update as needed. The `neper-commit` command should be used instead of `git commit` for all commits.

Please write good commit messages. A good commit message looks like this[1]:

```
Header line: explain the commit in one line (use the imperative),
50 characters max.

Body of commit message is a few lines of text, explaining things
in more detail, possibly giving some background about the issue
being fixed, etc etc.

The body of the commit message can be several paragraphs, and
please do proper word-wrap and keep columns shorter than about
74 characters or so. That way "git log" will show things
nicely even when it's indented.

Make sure you explain your solution and why you're doing what you're
doing, as opposed to describing what you're doing. Reviewers and your
future self can read the patch, but might not understand why a
particular solution was implemented.
```

C.2.5 Testing

The code can be tested using `CTest`. The usual way is as follows:

```
$ ctest
```

It is also possible to run only some of the tests.

- Option `-R` selects the tests whose name contains a character string:

  ```
  $ ctest -R string
  ```

[1] Mostly taken from Linus Torvalds's directives, `https://github.com/torvalds/subsurface-for-dirk/blob/a48494d2fbed58c751e9b7e8fbff88582f9b2d02/README#L88`. See also `https://chris.beams.io/posts/git-commit`.

As test names start by the letter of the module they refer to, followed by character '_', it becomes handy to run tests on a specific module, for example:

```
$ ctest -R T_
```

- Option `-E` selects the tests that do not contain a character string:

```
$ ctest -E string
```

- Option `-I` selects the tests from their numbers, for example:

```
$ ctest -I 3,5
```

Appendix D Versions

New in 4.0.2 (17 Sep 2020):
- module -V: fixed png output (disabled defective povray's version test).
- general: made minor improvements.

New in 4.0.1 (11 Sep 2020):
- module -T: added -transform unindex, fixed -morpho "file(tess_file)", improved -oriformat, made minor fixes.
- module -M: added col_stdtriangle and col_rodrigues mesh keys, fixed loading of pre-version 4 tessellations, fixed -meshface, made minor improvements.
- module -V: added -showvoidvox and -datavoidvoxcol, made minor fixes and code cleaning.
- documentation: made minor fixes and improvements.

New in 4.0.0 (30 Jul 2020):
- general: Neper now has a companion program for polycrystal plasticity, the new free / open-source finite element software package for polycrystal plasticity, FEPX (http://fepx.info), added new module -S for post-processing simulation results, added support for OpenMP on Mac.
- module -T: added option -group to (primarily) represent multiphase materials, added option -oridistrib to define in-cell orientation distributions, renamed orientation descriptors from e, ek, er, rtheta, R, q and g to euler-bunge, euler-kocks, euler-roe, axis-angle, rodrigues, quaternion and rotmat, changed default orientation descriptor to rodrigues, added support for active and passive orientation conventions to -oridescriptor, added circularity variable (as a synonym of sphericity), renamed tessellation key modeid into mode and lamid into lam, added tessellation key per, added options -stattess and -stattesr, made minor fixes.
- module -M: revised msh file content to include microstructure definition (element orientations, groups, etc.), element and node partitions, nsets and fasets, added options -statmesh, -statmesh0d, -statmesh1d, -statmesh2d, -statmesh3d and -statmeshco, updated per file, changed default value of -faset to all, improved -loadmesh, added format msh4 (msh version 4), added in-elset orientation distributions (as defined by -oridistrib in -T), added ori and bcs (optional FEPX) output files, added mesh key per, made .per output optional, cleaned code and made minor fixes.
- module -V: added simulation directory as generated by -S as input data, added -simstep, added VTK output, added ipf orientation coloring, changed default color map for real values to viridis (the previous one is available as 'legacy') and added many other colormaps using tinycolormap, fixed colors, added -datapointedgerad and -datapointedgecol, added -outdir, renamed -data*colscheme arguments for orientations, revised and extended -data options accordingly, made minor fixes.
- documentation: improved developer's guide, made minor fixes and improvements.

Note on backward (in)compatibility:
- module -T: renamed orientation descriptors (old tessellation files can be loaded, but option arguments must be updated), changed default orientation descriptor to rodrigues in all output files.
- module -M: changed nset and faset default values, added several fields to the msh file (those who have their own parser will need to update it), made .per

```
  output optional (use -format per to get it).
- module -V: changed default colormap for real values from
  blue,cyan,yellow,green to viridis, decreased average brightness.

New in 3.5.2 (12 Mar 2020):
- module -T: fixed -morphooptiobjective, fixed -statface nfaces, added
  tessellation keys nfaces_samedomain, nfacenb_samedomain, npolys_samedomain
  and npolynb_samedomain, fixed -transform planecut, added -transform
  crop(cube(...))  for tess, fixed tess loading, modified syntax of -transform
  crop for tesr, minor fixes.
- module -M: fixed meshing of tessellation cut by a sphere, fixed .per file for
  2nd-order meshing, fixed 2nd-order meshing with -interface discontinuous and
  cohesive, added -transform explode, added -statelt2d length, added -transform
  slice, fixed -statelt area for quad element, fixed -nset with discontinuous
  or cohesive (interface) mesh, added mesh keys, improved inp format, minor
  fixes.
- module -V: minor improvements.
- documentation:  minor fixes.

New in 3.5.1 (15 Nov 2019):
- module -T: fixed -morpho from wide grain size distributions, sped up -morpho
  tesr using openGJK, added olmap format.
- module -M: added -elt quad9, added -transform rotate, added fasets to .msh
  file, fixed -elt hex for non-cubic tessellations.
- module -V: fixed scale labels.
- general:  fixed compilation without openMP.

New in 3.5.0 (01 Oct 2019):
- module -T: added -transform slice and oriaverage,
  added new statistical distributions to -morpho:  beta, lorentzian, studentst,
  weibull, breitwigner, expnormal, moffat, pearson7, pseudovoigt and
  skewnormal, added endpoints to statistical distributions, added variable
  1-sphericity to -morpho, added tessellation keys, added -orioptilogvar,
  improved argument reading (multiscale tessellation), improved tesr format,
  improved -transform renumber, improved -ori fibre, improved -statcell
  convexity, replaced -transform plane with -transform hspace, fixed -loadtesr
  file.tesr:..., fixed -statvox e, fixed -for ori, fixed -domain, fixed -morpho
  centroidal, fixed tesr reading, fixed vtk output, enrich tesr file, made
  minor fixes.
- module -M: added -transform scale, translate and smooth, added
  -transporteltmethod, added -transportfepx, added mesh keys, added -performat,
  added kocks file to -for fepx:legacy, fixed -interface cohesive for Abaqus,
  fixed -elt hex, merged -scale into -transform, speed up -transport, made
  minor fixes.
- module -V: added -showvox, added -datavoxcol disori, added colour schemes
  R(), r, theta and rtheta, added -imageformat pov:objects, improved
  -includepov, fixed visualization of periodic meshes, made small fixes.
- documentation:  made minor fixes and improvements.
- general:  fixed compilation when GSL and NLopt locally installed, website now
  at http://neper.info.

New in 3.4.0 (15 Apr 2019):
```

- module -T: added tessellation cutting (to get non-convex domains) using -transform cut, added cell merging and removal using -transform mergecell and rmcell, added -transform resetcellid, added -ori spread, improved -morpho lamellar, improved -morpho diameq, added -format stl:bycell, added tessellation keys, fixed -morpho aspratio and rasterization of periodic tessellations, fixed -domain circle:split, made small fixes and improvements.
- module -M: made -interface mutliscale, renamed -mesh3dclconv into -mesh3dclreps, improved -cl, -rcl and -mesh3dclreps argument expressions, speed up -transport, fixed 2D remeshing, speed up -statelt and -statelset, added -[r]clface, -[r]cledge and -[r]clver.
- module -V: improved visualization of non-convex cells, fixed visualization of hex meshes, minor other fixes.

New in 3.3.0 (25 Jul 2018):
- New paper: "R. Quey, A. Villani, and C. Maurice. Nearly uniform sampling of crystal orientations. J. Appl. Crystallogr., vol. 51, doi:10.1107/S1600576718009019, 2018."
- module -T: added -ori uniform for uniform orientation distribution, added sister options -orioptiini, -orioptifix, -orioptistop and -orioptineigh, added -morpho tocta, columnar, bamboo and aspratio, fixed -morpho multimodal, improved -morphooptiini, added -transform translate, fixed tesr output for periodic tessellations, fixed tess to tesr conversion, added several tessellation keys, merged option -scale into -transform, made minor improvements.
- module -M: fixed meshing of periodic tessellation with openMP, allowed Gmsh development versions.
- module -V: improved camera parameters, fixed -slicemesh for hex meshes.

New in 3.2.0 (23 May 2018):
- general: Neper is now fully multithreaded.
- module -T: improved -morpho, added -morpho variable:value, added -morpho centroidtol, improved -morphooptiobjective, improved -transform crop, fixed -n from_morpho, added -transform addbuffer, renamed -datarpt* into -datavox*, added -transform renumber, added -domain stdtriangle, added **oridata to the tesr file, added -statvox, speed up tesr generation, added -morphooptilogtime val_ keys, minor fixes.
- module -M: improved inp format.
- module -V: improved msh reading, added -datapointrad arr, added -datavox options.
- documentation: small fixes.

New in 3.1.1 (20 Feb 2018):
- New paper: "R. Quey and L. Renversade, Optimal polyhedral description of 3D polycrystals: Method and application to statistical and synchrotron X-ray diffraction data, Comput. Methods Appl. Mech. Engrg., vol. 330, pp. 308-333, 2018."
- module -T: fixed -scale, added -domain rodrigues.
- module -M: fixed mesh of regularized tessellation through 2D-mesh pinches correction, fixed -stat when a tesr is meshed, improved -loadmesh, added -mesh2dpinchfix, added test on Gmsh's version.
- module -V : fixed -datapolyscale.

```
- general:  fixed use without nlopt or openmp.

New in 3.1.0 (05 Sep 2017):
- module -T: made all options applicable to multiscale tessellations,
  improved -morpho for all types of data, improved -morpho*
  options, added -n from_morpho to set the number of cells from all
  -morpho inputs, added -format stl, added -transform crop and 2d, added
  -morphooptilogtesr, added tessellation key 'scale', included openMP
  parallelization for -morpho tesr.
- module -M: allowed -interface cohesive -periodic in 2D, improved -dim
  for -format geof, improved -format geof, minor fixes.
- module -V: added -datapointrad tor and disc.
- documentation:  small fixes.
- general:  support OpenMP.

New in 3.0.2 (16 Feb 2017):
- module -T: added -transform scale and transform rotate for scalar
  tessellations (.tess), fixed -morpho with -periodic, fixed -morpho
  with non-unitary domains, fixed -statedge/-statface theta with
  -oricrysym hexagonal, improved -ori, added -morpho
  lamellar(v=crysdir), added ***tess/**cell/*crysym section to .tess
  file, fixed -morphooptialgo random, small fixes.
- module -M: fixed -interface cohesive in 2D and 3D (for Abaqus), enable
  -interface discontinuous and cohesive for periodic tessellations,
  added -format msh:binary, fixed faset internal for 3D, added
  -transport node:..., changed point keys "elt3d" and "elset3d" into "elt"
  and "elset" (now apply to 3D or 2D), small fixes.
- documentation:  minor fixes.

New in 3.0.1 (01 Dec 2016):
- module -T: fixed up options -periodic and -morphooptialgoneigh qsort,
  added tessellation key 'modeid' (for cells), added -morpho
  cube(N1,N2,N3) and -morpho square(N1,N2), enabled -loadtess -scale,
  added -oricrysym hexagonal, added tessellation keys 'nfacelist' and
  'theta', cleaned code, fixed documentation of .tess file, added tests
  on conflicing options.
- module -M: added option -scale, fixed hexahedral meshing of periodic
  tessellations, added physical groups to .msh, fixed 2D meshes in
  Abaqus (.inp) file, fixed up option -faset internal.
- module -V: fixed options -dataseed*.
- general:  removed libmatheval dependency, fixed testing.

New in 3.0.0 (12 Sep 2016):
- module -T: added 3 major capabilities:  (i) tessellation generation
  from morphological cell properties (options starting by -morpho),
  (ii) multiscale tessellation generation (using the ::  separator), and
  (iii) periodic and semi-periodic tessellation generation (option
  -periodic); made some other improvements and some clean up all over
  the place.
- module -M: added ability to mesh the new tessellations, including
  periodic tessellations; added interface meshing using cohesive
  elements (option -interface); made small other improvements.
```

```
- module -V: made small improvements.
- module -D: replaced by "make test" using CTest.
- new development website:  https://github.com/rquey/neper.

New in 2.0.5 (06 Feb 2016):
- module -T: fixed up -domain planes in 3D, added -domain sphere, added
  'rotate', 'translate' and 'scale' arguments to -domain, added normal
  specification in -morpho lamella, minor other improvements.
- module -M: fixed up vtk output.
- module -V: added -datacellcol id:filename, fixed up options -data*col
  id.
- module -D: minor improvements.

New in 2.0.4 (22 Jun 2015):
- module -T: fixed up regularization in 2D, extended -morpho planes to
  2D, added semi-periodicity for raster tessellations, minor fixes.
- module -M: fixed up 2D mesh output in Abaqus format, minor fixes.
- module -V: fixed up -datacellcolscheme, improved -cameracoo to account
  for the tessellation/mesh dimensions.

New in 2.0.3 (27 Nov 2014):
- module -M: fixed up bug on Mac OS X, fixed up Ctrl-C, fixed up and
  speed up option -statpoint 2dmesh*.
- module -T: improved options for 2-scale tessellations, added option
  '-clip'.

New in 2.0.2 (29 Sep 2014):
- module -T: fixed up regularization of cylinder tessellations, fixed up
  option '-domain planes', added tessellation cell domain, fixed up 3dec
  and ply support, added Wavefront obj format, added / fixed up
  tessellation keys.
- module -M: added vtk mesh format, fixed up fepx and geof mesh formats,
  added extrusion of a 2D mesh to get a 3D mesh (option -dim), fixed up
  topology reconstruction.
- module -V: added points plotting as cubes, spheres, cylinders or
  ellipsoids (options -showpoint and -datapoint*).

New in 2.0.1 (12 Mar 2014):
- Fixed up compilation on some systems, added support for libscotch
  version 6.0, small fixes and cleanups.
- module -T: enabled square and cube tessellations in .tess format,
  fixed up cell sorting, made option -id mandatory, improved
  regularization of 2D tessellations, added bunch of tessellation
  keys, small fixes.
- module -M: added 'domtype' mesh key.
- module -V: fixed up simultaneous tess and mesh printing, fixed up
  colouring based on id, improved camera positioning for 2D and 1D
  inputs, added coordinate system, improved option -slicemesh, added
  options -data*scaletitle, improved -data*scale options.

New in 2.0.0 (10 Jan 2014):
- General:  Full restructuring and added many new features.    Neper now
```

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  has 3 main modules:  tessellation module (-T), meshing module (-M) and
  visualization module (-V); details are provided below.  Added
  developer's guide and module (-D). Documentation has been much
  improved.
- module -T: added several tessellation algorithms (hardcore Voronoi
  and Laguerre Voronoi); added orientation generation (was previously in
  -O); significantly sped up tessellation; included and significantly
  sped up regularization (was previously in -FM); added 2-scale
  polycrystal generation; added 2D and 1D supports; improved statistics;
  enabled both scalar (tess) and raster (tesr) outputs; cleaned up tess
  file.
- module -M: module for free and mapped meshings (merging of -FM and
  -MM). Removed regularization (now in -T); added per-cell mesh size
  definition; sped up multimeshing; improved statistics.
- module -V: full restructuring; added support for 2D and 1D
  tessellations and meshes; the way all entities are shown (cells,
  polyhedra, faces, edges, vertices, germs, 3D/2D/1D/0D element sets and
  elements, nodes) can be set in great detail; added transparency.

New in 1.10.3 (26 Nov 2012):
- module -T: added 3dec geometry format, added option -checktess, minor
  improvements, added individual file extension support in -stattess,
  changed option -neigh 1 to -statp i,f,npl,fal,feql.
- module -FM: added 3dec geometry format; changed "top" and "bot" nset
  names for cylindrical domains to "z0" and "z1"; minor bug fixes;
  improved fev format support; added individual file extension support in
  options -stattess and -statmesh.
- module -O:  minor bug fixes.
- module -MM: sped up meshing; fixed -domain, -scale and -nset options,
  add .nper file for periodicity conditions; fixed msh output for meshes
  with different element dimensions; minor other bug fixes.
- module -VS: sped up meshing reconstruction and PNG file generation,
  added option '-camerasky', added option '-showeltedge', sped up mesh
  reconstruction, minor fixes
- documentation:  minor fixes.
- General:  minor fixes.

New in 1.10.2 (09 Aug 2012):
- module -T: fixed -centroid option.
- module -FM: fixed list of available meshing algorithms.    Added
  tests.
- module -MM: fixed nset syntax in inp (Abaqus) files.
- module -VS: added capability to plot mapped meshes.
- General:  various minor improvements, code cleaning.

New in 1.10.1 (08 June 2012):
- Bug fix to get Neper working after invoquing 'make install'.

New in 1.10.0 (04 June 2012):
- General:  New (hopefully simpler) installation procedure based on Cmake.
  Added support for domains of any convex polyhedral shape.
- module -VS: major code rewriting and option changes.  New capabilities
```

```
  for defining the colours and sizes of the tessellation / mesh
  (including gradients).    Added options to show only specific parts of the
  tessellation / mesh and to view slices of a mesh.  Other small
  enhancements.
- module -T : added option '-domain' to specify the shape of the domain
  (cuboidal, cylindrical or of any convex shape), small bug fixes, added
  centroid Voronoi tessellation generation (option -centroid), merged
  option -centrecoo into option -morpho, added polyhedron centroid
  coordinates in file .stt3, changed option -load to -loadtess, added
  output format '.ply' (thanks Ehsan!).
- module -FM: mesh partitionning needs libscotch version 5.1.12 or later,
  small bug fixes, changed default value of -faset to "" (i.e.  no faset
  in output), fixed bug for Abaqus output, added polyhedron centroid
  coordinates in file .stt3, added output format '.ply' (geometry only).
- module -MM: new options -dsize and -scale, new option -loadmesh, new
  option -outdim, changed arguments of -ttype, changed default value of
  -faset to "" (i.e.  no faset in output), fixed bug for Abaqus output,
  small bug fixes.

New in 1.9.2 (Sep 2011):
- module -T: added option -morpho for specifying the type of grain
  structure (equiaxed, columnar or bamboo), merged option -regular
  with -morpho, added post-processing -neighbour option for information
  on the polyhedron neighbours, added geo (Gmsh geometry) output format
  (mostly for visualization), fixed bugs.
- module -MM: proper processing of the input tess files, added msh
  (Gmsh) and inp (Abaqus) output formats, added options -morpho and
  -centrecoo (as in module -T), small bug fixes, code cleaning.
- module -FM: added geo (Gmsh geometry) output format (mostly for
  visualization), small bug fixes.
- documentation:  small corrections.

New in 1.9.1 (May 2011):
- module -FM: fixed bug occurring when -mesh3dalgo is not set by the
  user.    Small other bug fixes.
- module -MM: small bug fixes.

New in 1.9.0 (Apr 2011):
This is a major release.    Neper now has its own paper:
"R.Quey, P.R. Dawson and F. Barbe.    Large-scale 3D random polycrystal
 for the finite element method:  Generation, meshing and remeshing.
 Computer Methods in Applied Mechanics and Engineering,
 Vol.  200, pp.  1729--1745, 2011."
Please cite it in your works if you use Neper.
- General:  added option --rcfile to disregard / change the
  initialization file; big distribution and source clean up; bug fixes.
- module -T: added capability to generate regular morphologies
  (truncated octahedra), tess file format bumped to 1.9; big clean up.
- module -FM: included multimeshing, remeshing and mesh partitioning
  capabilities; big clean up.    Neper now uses the *standard* Gmsh
  distribution for 2D and 3D meshings (versions >=2.4.2).    Strongly
  reduced memory usage.
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- module -O: added capability to handle different orientation
  descriptors.
- module -VS: new visualization module to generate publication-quality
  images (PNG format) of the tessellations, meshes and more...

New in 1.8.1 (Aug 2009):
- upgraded website at http://neper.sourceforge.net
- module -T: new file format ***tess1.8, new option -restart to load an
  existing tessellation (not through std input any more), new option
  -printformat, bug fixes.
- module -MM: bug fixes.
- module -FM: new output format mae, new option -restart to restart from
  an existing geometry or mesh (options -mesh and -conv removed); new
  options -printformat and -maeextension; better mesh numbering (+ new
  options -elementfirstid and -nodefirstid), new way to choose the node
  sets to output (-nset 4), fixed option -estat, renamed -bwcy-clmin to
  -clmin, cleaned bunch of options, bug fixes.
- module -O: added option -eulerangleconvention (Bunge, Roe & Kocks);
  new output formats mae and geof (option -format).
- manual:  some corrections.

New in 1.8.0 (Jul 2009):
- First GPL-distributed version of Neper.
```

Appendix E GNU General Public License

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Version 3, 29 June 2007

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