

# Neper Reference Manual

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The documentation for Neper 1.10.0  
A 3D random polycrystal generator for the finite element method

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# Conditions of Use

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The precise conditions of the license for Neper are found in the General Public License that accompanies the source code (see [Appendix E \[GNU General Public License\], page 53](#)). Further information about this license is available from the GNU Project webpage <http://www.gnu.org/copyleft/gpl-faq.html>.

The Neper software package can be downloaded from <http://neper.sourceforge.net>. It has also two dedicated mailing lists,

- `neper-announce`: the “read-only” list for important news: new releases, bug fixes, etc. (low traffic, highly recommended!)

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- `neper-users`: the “read-write” list for users. Please send all questions, bug reports, requests or any errors or omissions in this manual to this list.

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The best way to get help is by sending a message to `neper-users@lists.sourceforge.net`. Note that you do not have to subscribe to the list to be able to send a message, nor to receive the reply. If you wish to contact the developer directly, use `rquey@users.sourceforge.net`.

## User Guidelines

If you use Neper for your own work, please cite it in your reports (books, papers, talks, ...). The Neper references are given below (if you do not wish to cite both, please cite the first one).

- *R. Quey, P.R. Dawson, F. Barbe. Large-scale 3D random polycrystals for the finite element method: Generation, meshing and remeshing. Computer Methods in Applied Mechanics and Engineering, vol. 200, pp. 1729–1745, 2011.*
- *Neper: a 3D random polycrystal generator for the finite element method (version 1.10), <http://neper.sourceforge.net>.*



# 1 Introduction

## 1.1 The Neper Project

### 1.1.1 Description

Neper is a 3D random polycrystal generator for the finite element method. It is built around several modules:

- Module -T is for generating polycrystal morphologies. They are described as space-filling tessellations of space whose vertices, edges, faces and volumes, represent the quadruple points, triple lines, grain boundaries and grains of the polycrystals, respectively. The polycrystal morphologies can be random Voronoi tessellations, or regular tessellations made of truncated octahedra. The tessellations are brick-shape by default, but can be of any convex shape. After they have been generated, they can be deformed to account for morphological texture.
- Module -FM aims at generating free (or “unstructured”) meshes of tessellations, that is, meshes comprised of tetrahedral elements that conform to the tessellation morphology. Neper includes several advanced features that are necessary to get good-quality meshes: optimized meshing rules, a geometry regularization approach, multimeshing (the competitive use of several meshers) and remeshing.
- Module -MM is for generating mapped meshes of tessellations. These meshes are comprised of regular hexahedral elements and so do not conform exactly to the tessellation morphology. Mapped meshes of standard tessellations, periodic tessellations and herein called *subdomain-type* tessellations can be created.
- Module -O provides crystallographic orientations for the grains. The orientations are randomly distributed according to a uniform distribution.
- Module -VS is for printing publication-quality images of the tessellations and meshes.

Neper aims 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. This makes it possible to automate all treatments.

### 1.1.2 Resources

Several, complementary resources describing the Neper capabilities are available:

- The Neper reference manual. It describes all the Neper capabilities. Each module is the subject of a specific chapter, in which all the available commands as well as the result files are described in detail. Some examples are also provided. The Neper documentation comes in two formats: a PDF file and an info file. Provided that the info file is properly installed at your site, it can be accessed by running the shell command: `info neper`.
- The Neper homepage: <http://neper.sourceforge.net>. It is where the Neper distribution can be downloaded from. It also provides an introduction to Neper, with some examples and illustrations.
- The Neper paper, “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.”, provides details on the algorithms. It can be downloaded from the Neper homepage or by following this link: [http://neper.sourceforge.net/neper\\_paper.pdf](http://neper.sourceforge.net/neper_paper.pdf).

## 1.2 Installing Neper

Neper is written in (mostly ANSI) C and can run on any Unix-like system. Neper can be compiled using Cmake, a standard open-source build system. The main steps are as follows,

- Create a ‘build’ directory, for example 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 ..
```

- To build and install Neper, then simply type,

```
$ make
```

```
$ make install (as root)
```

This will use the default configuration options, including on which dependencies are used, and should work out of the box provided that the required libraries are installed in standard system locations. A finer configuration can be achieved before building Neper, as described in the following.

### 1.2.1 Dependencies

Neper has mandatory as well as optional dependencies. Some dependencies are needed at compilation time. They are,

- the GSL library (mandatory)

It is likely to be available on your system or from your system package manager (packages `gsl` and `gsl-devel`). Alternatively, the source code version can be obtained from the GSL homepage, <http://www.gnu.org/software/gsl>.

- the libmatheval library (optional, *included* by default)

It is likely to be available on your system or from your system package manager (packages `libmatheval` and `libmatheval-devel`). Alternatively, the source code version can be obtained from the libmatheval homepage, <http://www.gnu.org/software/libmatheval>.

- the libScotch library (optional, *not included* by default)

Module -FM includes mesh partitioning capabilities, which make use of the Scotch mesh partitioner (version 5.1.12 or later). It can be downloaded from the Scotch homepage, [www.labri.fr/perso/pelegrin/scotch](http://www.labri.fr/perso/pelegrin/scotch).

Optional dependencies can be toggled on / off using Cmake’s GUI (`cmake-gui`) or `ccmake`, by setting variables `HAVE_LIBRARYNAME` to ON or OFF, respectively.

The following dependencies are not managed during the compilation. They are only needed at run time,

- the Gmsh program (mandatory for module -FM)

This version on Neper is intended to work with Gmsh (version 2.4.2 or later), which can be downloaded from <http://www.geuz.org/gmsh>. A working Gmsh installation must be available on your system.

- the POV-Ray program (mandatory for module -VS)

Module -VS uses POV-Ray to produce publication-quality images of the tessellations and meshes. POV-Ray can be downloaded from <http://www.povray.org>. POV-Ray must be available in the terminal through the command: `povray`.



## 1.3 Getting Started

Using Neper consists in running the command `'neper'` in a terminal, with a list of arguments,

```
$ neper list_of_arguments
```

The arguments define the problem for Neper to solve. Neper then returns output in ASCII files, together with some messages in the terminal. Neper includes some general-purpose self-explanatory commands,

```
$ neper --help
```

```
$ neper --version
```

```
$ neper --license
```

### 1.3.1 Call a Module

A typical Neper invocation consists in calling a module and providing it with a number of arguments:

```
$ neper module_name module_arguments
```

The module names are `'-T'`, `'-FM'`, `'-MM'`, `'-O'` and `'-VS'`. The module arguments can include both required input data and options. Options start by `'-'`. The options can be given in arbitrary order (except for module `-VS`) and are to be specified as follows: *"option\_name option\_value"*. The options can be written both in British English and in American English, although only the British English versions are indicated in this manual. String completion is available for all arguments, so they may be abbreviated as long as the abbreviation is not ambiguous. For example, in module `-O`, the option `'-descriptor'` can be abbreviated to `'-des'` or even safely to `'-d'`. Logical options can be selected by giving the value `'1'` or disabled by giving `'0'`. Neper is highly parametrable, and as a consequence includes quite a large number of options. For clarity sake, they are tagged according to their importance level in the reference manual: `'[Option]'` or `'[Secondary option]'`. The post-processing options are tagged `'[Post-processing]'`.

### 1.3.2 Initialization File

When Neper is started, it reads commands from an initialization file, `'$HOME/.neperrc'`, if that file exists. This behaviour can be modified through option `'--rcfile'`, which has to be loaded *prior to* calling a module,

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

To inhibit the reading of an initialization file, provide `'none'` as value of the *my\_file* argument.

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

An example of initialization file is given below:

```
neper comments -----
This is my default initialization file (~/.neperrc).
neper -FM -order 2 -maxff 20 -gmsh my_gmsh_path
      -rcl 0.8
neper -MM -order 2
neper comments -----
```

If `'neper module_name'` is not found, or if the initialization file is not found, Neper will just consider the command line arguments. Also, note that if an argument is initialized several times (for example, both in the initialization file and at the command line), the last specified value is retained.

### 1.3.3 Conventions

#### 1.3.3.1 Manual

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

1. A command that can be typed in a terminal is printed like **this**, or, in the case of a major command, like  
**\$ this**
2. a program (or command) option is printed like **'this'**;
3. The name of a variable is printed like **this**;
4. A metasyntactic variable (i.e. something that stands for another piece of text) is printed like *this*;
5. Literal examples are printed like **'this'**;
6. File names are printed like **'this'**.

#### 1.3.3.2 Option Arguments

When using the different Neper modules, you may want to provide several values to a given option. A typical example is when you want to set the format of the tessellation or mesh files. In this case, the several values can be specified at the same time, separated by commas. Neper will process them sequentially. For instance, in module -T, you may use option **'-format tess,ply'** to get the tessellation both in Neper's tessellation format **'tess'** and in Ply format **'ply'**.

## 2 Tessellation Generation: neper -T

Module -T enables one to generate Voronoi tessellations of a space *domain*. The domain can be cuboidal, cylindrical or of any other convex shape. The centres of the polyhedra can be randomly distributed in the domain, which leads to *random Voronoi tessellations* (also called *Poisson Voronoi tessellations*). It is also possible to generate columnar (2D) and bamboo (1D) grain morphologies, as well as regular, periodic, arrangement of polyhedra (truncated octahedra are currently available). It is also possible to generate centroidal Voronoi tessellations<sup>1</sup>, or even to load a user-defined distribution of centres. The tessellations can be scaled to generate morphological textures (flat or elongated grains). The module generates as output a tessellation file `‘.tess’` that describes exhaustively the polycrystal morphology (see [Appendix A \[File Formats\]](#), [page 43](#)). The `‘.tess’` file is an input file of the meshing modules, -FM and -MM (see [Chapter 3 \[Module -FM\]](#), [page 13](#) and [Chapter 4 \[Module -MM\]](#), [page 23](#)). Module -T also generates as output a `‘.oin’` file, which contains input data for the crystallographic orientation generation with module -O (see [Chapter 5 \[Module -O\]](#), [page 27](#)). The generated tessellation (`‘.tess’` file) can be visualized with module -VS ([Chapter 6 \[Module -VS\]](#), [page 31](#)).

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

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

===== N e p e r =====
Info  : A 3D random polycrystal generator for the finite element method
Info  : Version 1.10.0
Info  : (compiled with: gsl libmatheval)
Info  : Loading initialization file ‘/home/rquey/.neperrc’...
Info  : -----
Info  : MODULE -T loaded with arguments:
Info  : [ini file] (none)
Info  : [com line] -n 10 -id 1
Info  : -----
Info  : Reading input data ...
Info  : Creating domain ...
Info  : Creating polyhedron centres ...
Info  : Creating tessellation ...
Info  : Writing results ...
Info  :      [o] Writing file ‘n10-id1.tess’ ...
Info  :      [o] Wrote file ‘n10-id1.tess’.
Info  :      [o] Writing file ‘n10-id1.oin’ ...
Info  :      [o] Wrote file ‘n10-id1.oin’.
Info  : Elapsed time: 0.004 secs.
=====
```

<sup>1</sup> Q. Du, V. Faber and M. Gunzburger, Centroidal Voronoi Tessellations: Applications and Algorithms, SIAM Review, 41, 637–676, 1999.

## 2.1 Arguments

### 2.1.1 Input Data

By default, the domain to tessellate is taken as a cube of unit size. For defining another domain, see option ‘`-domain`’.

`-n integer` [Input data]

Number of polyhedra of the tessellation, except for regular morphologies (truncated octahedra, etc., see option ‘`-morpho`’ for details).

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

`-id integer` [Input data]

Identifier of the tessellation.

Possible values: *any*. Default value: *random*.

`-morpho char_string` [Input data]

Type of morphology of the polyhedra. For random Voronoi tessellations, it can be either equiaxed (*equiaxed*), columnar (*columnar*{*x,y,z*}) or bamboo-like (*bamboo*{*x,y,z*}).

To load a particular set of polyhedron centres, use the syntax ‘*@file\_name*’ where *file\_name* is the name of a file containing the  $3 * n$  coordinates.

Regular morphologies can also be obtained: truncated octahedra (*tocta*), in which case the value of option ‘`-n`’ stands for the number of polyhedra along an edge of the domain instead of the total number of polyhedra.

Possible values: *see above list*. Default value: *equiaxed*.

`-centroid logical` [Input data]

Use this option to turn the tessellation centroidal.

Possible values: 0 or 1. Default value: 0.

The generation of a centroidal Voronoi tessellation is based on Lloyd’s algorithm and can be two to three orders of magnitude as long as for the equivalent Voronoi tessellation. The convergence criteria can be adjusted using options ‘`-centroidfact`’, ‘`-centroidconv`’ and ‘`-centroiditermax`’.

Is it also possible to load a 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*.

### 2.1.2 General Options

`-o file_name` [Option]

Specify the output file name.

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

### 2.1.3 Domain Options

`-domain char_string ...` [Option]

Specify the type of domain and its size. For a cuboidal shape, provide ‘*cube*’ followed by the sizes along the *x*, *y* and *z* directions. For a cylindrical shape, provide ‘*cylinder*’ followed by the height and diameter. For a tessellation polyhedron, provide ‘*tesspoly*’ followed by the name of the tessellation file (‘*.tess*’) and the number of the polyhedron (the tessellation must not be regularized). For an arbitrary shape, provide ‘*planes*’ followed by the name of a file containing the total number of planes then, for each plane, the parameters of its equation

( $a$ ,  $b$ ,  $c$  and  $d$  for an equation of the form  $ax + by + cz = d$ ). The plane normal must be an outgoing vector of the polyhedron.

Possible values: **see above list**. Default value: **cube 1 1 1**.

**-cylinderfacet integer** [Secondary option]

Specify the number of facets along the circular part of a cylindrical domain.

Possible values: **any**  $\geq 3$ . Default value: **function of the poly rad**.

## 2.1.4 Tessellation Options

**-scale real real real** [Option]

Specify the factors in the x, y and z directions by which the tessellation is to be scaled (once generated).

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

**-sort char\_string char\_string** [Secondary option]

This option can be used to sort the tessellation entities (typically to facilitate data post-processing). The first argument is the type of entity to sort (must be **poly**) and the second argument is the mathematical expression used for sorting (see [Appendix B \[Mathematical Expressions\]](#), page 47). For polyhedra, the available variables are the centre coordinates, *cenx*, *ceny* and *cenz*, the true and body parameters *true* and *body*, and the volume *vol*.

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

**-randomize real integer** [Secondary option]

This option can be used to “randomize” the coordinates of the polyhedron centres. Provide as argument the maximum shift distance and an identifier for the randomization. The resulting centre shift distances are uniformly distributed between 0 and the maximum shift distance.

Possible values: **any**  $> 0$  **any**. Default value: **none**.

**-randomizedir char\_string** [Secondary option]

This option can be used with option ‘**-randomize**’, to specify the possible directions in which the polyhedron centres are to be shifted. Provide as argument the directions. Combine them with ‘,’.

Possible values: **x**, **y**, **z**. Default value: **x,y,z**.

**-centroidfact real** [Secondary option]

This option can be used with option ‘**-morpho centroid**’, to specify the factor by which the germ positions are shifted between their current positions and the centroid positions, at each iteration. (Lloyd’s algorithm is obtained for a value of 1, but a lower value can lead to faster convergence.)

Possible values: **0** to **1**. Default value: **0.5**.

**-centroidconv real** [Secondary option]

This option can be used with option ‘**-morpho centroid**’, to specify the maximum tolerance on the distance between the polyhedron centres and centroids. The tolerance is relative to the average grain radius.

Possible values: **any**  $> 0$ . Default value: **0.02**.

**-centroiditermax integer** [Secondary option]

This option can be used with option ‘**-morpho centroid**’, to specify the maximum number of iterations. You should consider using option ‘**-centroidconv**’ instead.

Possible values: **any**. Default value: **1000**.

### 2.1.5 Output Options

**-format** *char\_string* [Option]  
 Specify the format of the output file(s). The available formats are the Neper **tess** and **oin**, the Gmsh **geo** and the Ply **ply** (combine with commas).  
 Possible values: **tess**, **oin**, **geo**, **ply**. Default value: **tess,oin**.

### 2.1.6 Post-Processing Options

**-stat** *logical* [Post-processing]  
 Provide statistics on the tessellation.  
 Possible values: 0 or 1. Default value: 0.  
 Result file: extension '**.stt#**'.

**-neighbour** *logical* [Post-processing]  
 Provide a file with information on the first neighbours of the polyhedra.  
 Possible values: **any**. Default value: **none**.  
 Result file: extension '**.neigh**'.

**-pointpoly** *file\_name* [Post-processing]  
 Provide the numbers of the polyhedra of which specific points belong. Give as argument the name of the file containing the coordinates of the points.  
 Possible values: **any**. Default value: **none**.  
 Result file: extension '**.polyid**'.

## 2.2 Output Files

### 2.2.1 Tessellation

- Neper-native tessellation file: '**.tess**'  
 It contains an exhaustive description of the tessellation. See [Appendix A \[File Formats\]](#), [page 43](#) for the file syntax.
- 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 visualization. (Note that you can even get a mesh of the tessellation out from Gmsh, but it will be of lower quality than by using module **-FM**.)
- Ply file: '**.ply**'  
 It contains a description of the tessellation written under the standard "Polygon File Format" '**.ply**'.

### 2.2.2 Orientation

- orientation input file: '**.oin**'  
 It contains data for generating the grain orientations, and is an input file for module **-O** (see [Chapter 5 \[Module -O\]](#), [page 27](#)).

### 2.2.3 Statistics

Several files are provided for statistics on tessellations, whose formats are provided below. All files are formatted with one entity (vertex, edge, face or polyhedron) per line.

- tessellation vertex statistics, '**.stt0**': *id true body state x y z*
- tessellation edge statistics, '**.stt1**': *id true body state length*

- tessellation face statistics, `‘.stt2’`: *id true body state ver\_qty area ff*
- tessellation polyhedron statistics, `‘.stt3’`:  
*id true body state x y z ver\_qty edge\_qty face\_qty vol xc yc zc*

*xc*, *yc* and *zc* denote the centroid (centre of mass) coordinates.

## 2.2.4 Post-Processing

- polyhedron identifier file: `‘.polyid’`

It contains the identifiers of the polyhedra of which specific points belong (see option `‘-pointpoly’`). By definition, they range from 1 to the maximum number of polyhedra in the tessellation. In the case of a point which does not belong to any polyhedron, the returned value is 0.

- polyhedron neighbours file: `‘.neigh’`

It contains information on the neighbours of the polyhedra. The file is formatted with one polyhedron per line, with the following entries: *id neighbour\_qty neighbour1\_id neighbour2\_id ... neighbour1\_facearea neighbour2\_facearea ... neighbour1\_faceeq neighbour2\_faceeq ...*. *neighbour#\_id* is a positive integer, except for a polyhedron face which belongs to the boundary of the domain (in this case, the value ranges between  $-6$  and  $-1$ ). A face equation is specified by the parameters *d*, *a*, *b* and *c* (in this order), with the equation being:  $ax + by + cz = d$ . The vector  $(a, b, c)$  is pointing outwards of the polyhedron.

## 2.3 Examples

Below are some examples of use of neper -T. Illustrations can be found at [http://neper.sourceforge.net/neper\\_t.html](http://neper.sourceforge.net/neper_t.html).

1. Generate a polycrystal made of 100 grains, with identifier = 1.  
`$ neper -T -n 100 -id 1`
2. Use an elongated domain and generate a polycrystal made of 100 grains, with identifier = 1.  
`$ neper -T -n 100 -id 1 -domain cube 3 1 0.33`
3. Generate a polycrystal made of 100 grains, with identifier = 1, and stretch it to model a morphological texture.  
`$ neper -T -n 100 -id 1 -scale 3 1 0.33`
4. Generate a polycrystal made of 100 columnar grains.  
`$ neper -T -n 100 -id 1 -morpho columnarz`
5. Generate a polycrystal made of approximately 5x5x5 truncated octahedra.  
`$ neper -T -n 5 -morpho tocta`
6. Generate a polycrystal made of 100 grains in a cylindrical domain of height 2 and diameter 1.  
`$ neper -T -n 100 -id 1 -domain cylinder 2 1`





### 3 Tessellation Free Meshing: neper -FM

Module -FM is the module to generate a free mesh of a tessellation, that is, a mesh comprised of tetrahedral elements that conform to the tessellation morphology. The aim is to generate a mesh into elements of size as close as possible to a desired target value, and of high quality, that is, of equilateral shape. The input file is a tessellation file (‘.tess’), as provided by module -T. The output mesh can be written in several formats.

Several options are available for specifying the desired mesh properties. The target element size of the mesh can be specified through the following parameters:

- The *characteristic length* (c1). It corresponds to the target size of the elements. This size is the length of a line element (1D), and the length of the edge of a triangle element (2D) and of a tetrahedral element (3D). For convenience, a value relative to the average polyhedron size, *rc1*, is also defined:  $rc1 = 2 * c1 / (\text{average\_poly\_volume})^{1/3}$ .

For ensuring mesh quality to the greatest extent possible, Neper includes several advanced capabilities:

- Geometry regularization. It consists in removing the small features of the tessellation (the edges and faces), which are smaller than the target element size and as a consequence would need local mesh over-refinements. Using this capability is done by allowing some level of geometrical distortion, the face *flatness fault*, through option ‘-maxff’ (value in degree).
- Multimeshing. Each tessellation face and volume is meshed separately of the others, with several meshing algorithms, and to the mesh of best quality is retained. This is needed for meshing Voronoi tessellations, and has the advantage of ensuring meshing robustness and optimizing mesh quality. This is controlled by options ‘-mesh2dalgo’ and ‘-mesh3dalgo’.
- Remeshing can also be applied to generate a new, good-quality mesh on a mesh containing poor-quality elements (options starting by ‘-remesh’). The variables defined on the old mesh can be transported on the new mesh (options starting by ‘-transport’).

Mesh partitioning capabilities enable to divide the mesh nodes and elements into several sets while minimizing the interfaces between them<sup>1</sup>, for parallel finite element calculations. Partitioning can return any number of partitions, or more efficiently, can be carried out according to a given parallel computer architecture, in which case the number of partition must be a power of 2 (options starting by ‘-part’).

In the output mesh, the individual entities of the tessellations (the volumes, the faces, the edges and the vertices) are described by element sets (option ‘-outdim’). Node sets of the faces, the edges and the vertices of the surface of the tessellation are also provided for prescribing the boundary conditions (option ‘-nset’). The surface element sets (triangles) are also provided (option ‘-faset’). The mesh order can be 1 or 2, corresponding to 3-node tetrahedral elements and 10-node tetrahedral elements, respectively (option ‘-order’). Statistical data can be obtained on the properties of the tessellations and meshes (options starting by ‘-stat’).

Options are also available to work on an existing mesh (options starting by ‘-loadmesh’).

---

<sup>1</sup> Each partition being assigned to a processor in the finite element calculation, the minimization of the interfaces between the partitions is done in terms of the number of necessary communications between processors.

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

```
$ neper -FM n10-id1.tess -maxff 20
```

```
===== N e p e r =====
Info  : A 3D random polycrystal generator for the finite element method
Info  : Version 1.10.0
Info  : (compiled with: gsl libmatheval)
Info  : Loading initialization file '/home/rquey/.neperrc'...
Info  : -----
Info  : MODULE -FM loaded with arguments:
Info  : [ini file] -nset faces -mo 2 -gmsh /home/rquey/bin/gmsh -surf z1
Info  : -partrenumber 1
Info  : [com line] n10-id1.tess -maxff 20
Info  : -----
Info  : Reading input data ...
Info  :   - Reading arguments ...
Info  : Creating geometry ...
Info  :   - Loading tessellation ...
Info  :     [i] Parsing file 'n10-id1.tess' ...
Info  :     [i] Parsed file 'n10-id1.tess'.
Info  :   - Regularizing tessellation ... (sel = 0.12)
Info  :     > loop    length    deleted
Info  :     >   1      100%         16
Info  :     >   2      100%          0
Info  : Meshing ... (cl = 0.232, pl = 2)
Info  :   - Preparing ... 100%
Info  :   - 0D meshing ... 100%
Info  :   - 1D meshing ... 100%
Info  :   - 2D meshing ... 100% (0.26|0.85/16%|83%)
Info  :   - 3D meshing ... 100% (0.89|0.91/100%| 0%)
Info  :   - Switching mesh to order 2 ...
Info  :   - Searching nsets ...
Info  : Writing mesh results ...
Info  :   - Preparing mesh ...
Info  :   - Mesh properties:
Info  :     > Node number:    1852
Info  :     > Elt  number:    1041
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: 13.353 secs.
=====
```

## 3.1 Arguments

### 3.1.1 Input Data

In normal use, the input data is a tessellation file:

***file\_name*** [Input data]  
 Name of the tessellation file.  
 Possible values: **any**. Default value: **none**.

It is also possible to load a mesh from a file. (Using option ‘-o’ along with this capability avoids overwriting the input data.)

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

**-loadmeshnodecoo *file\_name*** [Input data]  
 Overwrite the node coordinates. The file must contain the list of coordinates (3 real values per node).  
 Possible values: **any**. Default value: **none**.

### 3.1.2 General Options

**-gmsh *full\_path\_name*** [Requirement]  
 Specify the *full* path of the Gmsh binary.  
 Possible values: **any**. Default value: **/usr/local/bin/gmsh**.

**-o *file\_name*** [Option]  
 Specify output file name.  
 Possible values: **any**. Default value: **none**.

### 3.1.3 Geometry Regularization Options

A non-zero value of *maxff* is necessary to enable geometry regularization; the other options are for fine tuning.

**-maxff *real*** [Option]  
 Maximum face flatness fault which is allowed (in degree).  
 Possible values: 0 to 180 (**recommended: 20**). Default value: 0.

**-sel or -rsel *real*** [Secondary option]  
 Absolute or Relative Small Edge (maximum) Length. The relative small edge length is defined relative to the default value. By default, **sel** is set so as to avoid mesh over-refinement (**c1/p1**). Use this option if you want to choose a different length.  
 Possible values: **any**. Default value: **-sel c1/p1**.

**-mloop *integer*** [Secondary option]  
 Maximum number of edge deletion loops.  
 During each loop, the small edges are considered in turn from the shortest to the largest. One loop already leads to very satisfactory results. Use more to get better results. The deletion process completes as soon as no edges are deleted within a loop.  
 Possible values: **any**. Default value: 2.

### 3.1.4 Meshing and Multimeshing Options

- cl or -rcl *real*** [Option]  
 Absolute or relative characteristic length of the elements. **rcl** is defined relative to the average polyhedron volume. The default **-rcl 1** leads to a mesh density of about 100 tetrahedral elements per grain.  
 Possible values: **any**. Default value: **-rcl 1**.
- dim *integer*** [Option]  
 Specify the mesh dimension.  
 Possible values: 0 to 3. Default value: 3.
- order *integer*** [Option]  
 Specify the mesh order.  
 Possible values: 1 or 2. Default value: 1.
- pl *real*** [Secondary option]  
 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.
- cl3 or -rcl3 *real real real*** [Secondary option]  
 Absolute or relative characteristic length of the elements in the x, y and z directions. **rcl3** is defined relative to the average polyhedron volume. Note that options '**-[r]cl**' and '**-[r]cl3**' are mutually exclusive.  
 Possible values: **any**. Default value: **none**.
- clmin *real*** [Secondary option]  
 Minimum characteristic length of the elements. Using this option is not recommended.  
 Possible values: **any**. Default value: **none**.

The following options define the 2D and 3D-meshing algorithms. The algorithms have the format '**mesh**' or '**mesh/opti**', where **mesh** and **opti** stand for the meshing and optimization algorithms and are 4-character long. *Multimeshing* can be used by providing several algorithms combined with commas, e.g. **mesh1/opti1,mesh1/opti2,mesh2/opti2**. The 2D and 3D meshings are carried out using the Gmsh<sup>1</sup> and Netgen<sup>2</sup> libraries (see the Gmsh reference manual for information on the algorithms).

For 2D meshing, the available values of **mesh** are **made** (MeshAdapt+Delaunay), **mead** (MeshAdapt), **dela** (Delaunay) and **fron** (Frontal). There is no optimization. The default is **fron,made** and it is recommended to retain multimeshing in use for meshing robustness sake. For 3D meshing, the available values of **mesh** are currently limited to **netg** (Netgen). The available values of **opti** are **gmsh** (Gmsh), **netg** (Netgen) and **gmne** (Gmsh+Netgen). For convenience, two generic entries are also defined. The entry **default**, which is the default value, provides a good balance between mesh quality and computation time. The entry **qualmax** provides the best results on mesh quality (full use of multimeshing). The values of **default** are **fron,made** for the 2D case and **netg/gmsh,netg/gmne** for the 3D case. The values of **qualmax** are **made,mead,dela,fron** for the 2D case and **netg/gmsh,netg/netg,netg/gmne** for the 3D case.

<sup>1</sup> 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.

<sup>2</sup> J. Schöberl, Netgen, an advancing front 2d/3d-mesh generator based on abstract rules. Comput. Visual. Sci., 52, 1–41, 1997.

- mesh2dalgo *char\_string*** [Option]  
Specify the 2D meshing algorithm. Multimeshing is allowed by providing several algorithms, (combine with commas).  
Possible values: `made`, `mead`, `dela`, `fron`,.. Default value: `default (= fron,made)`.
- mesh3dalgo *char\_string*** [Option]  
Specify the 3D meshing algorithm. Multimeshing is allowed by providing several algorithms, (combine with commas).  
Possible values: `netg`, `netg/netg`, `netg/gmsh`, `netg/gmne`,.. Default value: `default (= netg/gmsh,netg/gmne)`.
- mesh3doptiexpr *string*** [Secondary option]  
Specify the value of *O* for the multimeshing optimization, as a function of *Odis* and *Osize* (see the Neper paper).  
Possible values: `any`. Default value: `Odis^0.8*Osize^0.2`.
- mesh3doptidisexpr *string*** [Secondary option]  
Specify the value of *Odis* for the multimeshing optimization, as a function of the element distortion parameter *dis* (see the Neper paper).  
Possible values: `any`. Default value: `dis^(exp((dis^0.1)/(dis^0.1-1)))`.

### 3.1.5 Domain Boundary Meshing Options

These options are for specifying geometry regularization and meshing conditions for the polyhedra at the domain boundary different than those that apply to the inner polyhedra. This is useful for coarsening the meshes of the boundary grains when they are disregarded in the analysis due to possible boundary effects. The domain boundary polyhedra can be defined using the following variables:

- **body**: the minimum number of polyhedra between the considered polyhedron and the domain boundary. Its value is 0 for polyhedra intersecting the domain boundary, and increases with the distance to the domain boundary.
- **true**: a polyhedron is said to be *true* if its shape is not biased by the domain boundary. This requires the polyhedron not to be cut by the domain boundary, but actually the condition is a bit more restrictive. The value of **true** is an integer equal to 0 for polyhedra which do not match the above-mentioned criterion, and higher values otherwise. For the latter cases, the value of **true** is defined to be equal to *n* for true polyhedra surrounded by polyhedra whose value of **true** is higher than or equal to (*n* - 1). This definition is consistent with the one of the **body** variable, in terms of how the values of neighbouring grains compare. As for **body**, the value of **true** increases with the distance to the domain boundary, but typically  $true \leq body$ .

- dbound *char\_string*** [Option]  
Define which polyhedra belong to the domain boundary. The expression can be based on the following arguments: **body** and **true**. An example is `"body<=1"`.  
Possible values: `any`. Default value: `none`.
- dboundcl and -dboundrcl *real*** [Option]  
Absolute or relative characteristic length of the elements at the domain boundary. **rcl** is defined relative to the average polyhedron volume.  
Possible values: `any`. Default value: `none`.
- dboundsel and -dboundrsel *real*** [Secondary option]  
Absolute or Relative Small Edge (maximum) Length at the domain boundary. The relative small edge length is defined relative to the default value. By default, **sel** is set so as to avoid

mesh over-refinement ( $c1/p1$ ). Use this option if you want to choose a different length.  
Possible values: **any**. Default value: **-sel c1/p1**.

**-dboundpl** *real* [Secondary option]  
Progression factor for the element characteristic lengths. This value is the maximum ratio between the lengths of two adjacent 1D elements.  
Possible values: **any**  $\geq 1$ . Default value: 2.

### 3.1.6 Mesh Partitioning Options

Mesh partitionning is achieved through the libScotch library<sup>3</sup>. In Neper, The two following options enable to turn on mesh partitioning; they are mutually exclusive,

**-partqty** *integer* [Option]  
Use this option to specify the quantity of partitions.  
Possible values: **any**. Default value: 0.  
Result file: extension '**[e,n]part**'.

**-partarchfile** *file\_name* [Option]  
Use this option to specify the architecture of the target machine. Give as argument the name of the file describing the architecture.  
Possible values: **any**. Default value: **none**.  
Result file: extension '**[e,n]part**'.

Here are additional options,

**-partbalancing** *real* [Secondary option]  
Use this option to set the level of partition balancing (0: none, 1:full). This is a highly CPU-sensitive capability (full balancing requires a lot of time).  
Possible values: 0 to 1. Default value: 0.5.

**-partmethod** *char\_string* [Secondary option]  
Specify the partitioning method, expressed in Scotch's jargon.  
Possible values: **any** (including **none**). Default value: **see\_the\_source**.

**-partrenumbering** *logical* [Secondary option]  
Use this option to renumber the nodes and elements according to partitioning.  
Possible values: 0 or 1. Default value: 0.

**-partsets** *logical* [Secondary option]  
Use this option to print the partitions as nsets and elsets in the mesh file (**geof** format only).  
Possible values: 0 or 1. Default value: 1.

### 3.1.7 Remeshing Options

**-remesh** *file\_name* [Option]  
Use this option for remeshing a mesh. Provide as argument the mesh file.  
Possible values: **any**. Default value: **none**.

**-remeshtess** *file\_name* [Option]  
Use this option to specify a tessellation associated to the mesh to remesh. This can be useful, for example, when the meshed domain is not a regular box, to determine the node sets.  
Provide as argument the tessellation file.  
Possible values: **any**. Default value: **none**.

<sup>3</sup> F. Pellegrini, Scotch and libScotch 5.1 User's Guide, INRIA Bordeaux Sud-Ouest, ENSEIRB & LaBRI, UMR CNRS 5800, 2008.

**-transport** *file\_name integer char\_string char\_string file\_name* [Option]

...

Use this option for transporting data from a parent mesh to a child mesh (typically obtained by remeshing). First provide the name of the parent mesh file. The child mesh is taken as the result mesh (usually obtained by remeshing, but it can also be loaded with ‘-loadmesh’). Then provide as argument the number of different data to transport; then, for each of them, **elt** (mandatory), the type of data (under the format **[integer,real]X**, where **X** is the dimension) and the name of the file containing the parent data.

Possible values: **any**. Default value: 0.

**-transporttess** *file\_name* [Option]

Use this option to specify a tessellation associated to the mesh from which the data are transported. This is not mandatory. Provide as argument the tessellation file.

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

### 3.1.8 Output Options

**-outdim** *char\_string* [Option]

Specify the dimensions of the mesh to output. It can go from 0 to 3, for point to volume elements (combine with commas).

Possible values: 0, 1, 2, 3,. Default value: 0,1,2,3.

**-format** *char\_string* [Option]

Specify the format of the output file(s). For the mesh, the available formats are: **msh** for Gmsh, **abq** for Abaqus, **geof** for Zset/Zébulon, and **fev** for Fem-Evps. For the tessellation geometry, the available formats are: **tess** and **geo**. Combine arguments with commas.

Possible values: **anyone of the above list**. 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. To get the nset corresponding to individual entities, provide their names, that is, for a cubic domain, **[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. Append ‘**body**’ to the name to get only the body nodes of the sets. Combine them with commas.

Possible values: **any**. Default value: **faces**.

**-facet** *char\_string* [Option]

Specify the domain surfaces to provide. Use ‘**faces**’ for all faces. Combine them with commas. Possible values: **faces**, **[x-z] [0,1]** (for a cubic domain). Default value: **none**.

### 3.1.9 Post-Processing Options

**-stattess** *logical* [Post-processing]

Provide statistics on the tessellation.

Possible values: 0 or 1. Default value: 0.

Result file: extension ‘**.stt#**’.

**-statmesh** *logical* [Post-processing]

Provide information and statistics on the elements and element sets.

Possible values: 0 or 1. Default value: 0.

Result file: extension ‘**.stm#**’.



### 3.1.10 Advanced Options

These advanced options set running conditions for the mesher.

- `-mesh2dmaxtime` *real* [Secondary option]  
Maximum processing time allowed to the mesher for meshing a tessellation face (in seconds).  
Possible values: **any**. Default value: 1000.
- `-mesh2drmaxtime` *real* [Secondary option]  
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]  
Maximum iterations in 3D meshing for a particular face (in case of failure).  
Possible values: **any**. Default value: 3.
- `-mesh3dmaxtime` *real* [Secondary option]  
Maximum processing time allowed to the mesher for meshing a tessellation volume (in seconds).  
Possible values: **any**. Default value: 1000.
- `-mesh3drmaxtime` *real* [Secondary option]  
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]  
Maximum iterations in 3D meshing for a particular volume (in case of failure).  
Possible values: **any**. Default value: 3.
- `-mesh3dc1conv` *real* [Secondary option]  
Maximum tolerated difference between the characteristic length `c1` and the average element length (for each polyhedron). Neper tries its best to get the average element size to match `c1`. Use this option to change the tolerance on the relative difference between the two. This is a highly CPU-sensitive capability (using a high value can be an efficient way to speed up meshing).  
Possible values: **any**. Default value: 0.02.

## 3.2 Output Files

### 3.2.1 Mesh

The mesh can be written in the following formats:

- Gmsh format: file ‘`.msh`’
- Abaqus format: file ‘`.inp`’
- Zset/Zébulon format: file ‘`.geof`’
- Fem-Evps format: files ‘`.parms`’, ‘`.mesh`’, ‘`.surf`’, ‘`.opt`’ and ‘`.bcs`’

The following files are for describing the partitions:

- Node partition description, file ‘`.npart`’: *node\_id partition\_id*. The partition identifier ranges from 1 to the total number of partitions.
- Element partition description, file ‘`.epart`’: *elt\_id partition\_id*. The partition identifier ranges from 1 to the total number of partitions.
- Remeshing file, ‘`.rem`’: *elt\_id corresponding\_old\_elt\_id*.



### 3.2.2 Tessellation

- Neper-native tessellation file: `‘.tess’`  
It contains an exhaustive description of the tessellation. See [Appendix A \[File Formats\]](#), [page 43](#) for the file syntax.
- 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 visualization. If the tessellation has been regularized, Gmsh will complain about surfaces not being plane, but for visualization this can be disregarded. (Note that you can even get a mesh of the tessellation out from Gmsh, but it will be of lower quality than by using module -FM.)
- Ply file: `‘.ply’`  
It contains a description of the tessellation written under the standard “Polygon File Format” `‘.ply’`.

### 3.2.3 Statistics

Several files are provided for statistics on tessellations, whose formats are provided below. All files are formatted with one entity (vertex, edge, face or polyhedron) per line.

- Tessellation vertex statistics, `‘.stt0’`: *id true body state x y z*
- Tessellation edge statistics, `‘.stt1’`: *id true body state length*
- Tessellation face statistics, `‘.stt2’`: *id true body state ver\_qty area ff*
- Tessellation polyhedron statistics, `‘.stt3’`:  
*id true body state x y z ver\_qty edge\_qty face\_qty vol xc yc zc*

*xc*, *yc* and *zc* denote the centroid (centre of mass) coordinates.

The following are for statistics on the mesh.

- Mesh non-quality statistics file, `‘.stm1’`: *id elset\_id true vol mean\_length x y z*.
- Mesh quality statistics file, `‘.stm2’`: *id elset\_id true radius\_ratio angle\_min*.

## 3.3 Examples

Below are some examples of use of neper -FM. Illustrations can be found at [http://neper.sourceforge.net/neper\\_fm.html](http://neper.sourceforge.net/neper_fm.html).

1. Mesh tessellation n100-id1.tess.  

```
$ neper -FM n100-id1.tess
```
2. Mesh tessellation n100-id1.tess using geometry regularization.  

```
$ neper -FM n100-id1.tess -maxff 20 -sel 0.05
```
3. Mesh tessellation n100-id1.tess with a mesh size of  $rcl = 0.5$  and in 2nd-order elements.  

```
$ neper -FM n100-id1.tess -maxff 20 -sel 0.05 -rcl 0.5 -order 2
```
4. Mesh tessellation n100-id1.tess with small elements for the inner grains and bigger elements for the surface grains.  

```
$ neper -FM n100-id1.tess -maxff 20 -rcl 0.2 -dbound "body==0"
-dboundrcl 0.5 -dboundsel 0.05
```
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 -FM -remeshtess n150.tess -remesh n150_def.msh -transport
n150_def.msh 1 elt real1 n150_def.data -rcl 0.5 -o n150_new
```

Below are some examples of advanced use.

1. *Multimeshing.* Improve mesh quality as far as possible through 3D multimeshing.  

```
$ neper -FM n10-id1.tess -maxff 20 -rcl 0.8 -order 2
  -format tess,msh,abq -o n10
  -mesh3dalgo netg/gmsh,netg/netg,netg/gmne
```
2. *Mesh partitionning.* Like 2., but partition in 8 partitions and renumber the nodes and elements accordingly.  

```
$ neper -FM n10-id1.tess -maxff 20 -rcl 0.8 -order 2
  -format tess,msh,abq -o n10
  -partq 8 -partrenum 1
```
3. *Orthotropic mesh refinement.* Mesh tessellation ‘n10-id1.tess’ with different element characteristic lengths along x, y and z:  $rcl = 1$ ,  $rcl = 0.5$  and  $rcl = 0.25$ , respectively. Use geometry regularization.  

```
$ neper -FM n10-id1.tess -rcl3 1 0.5 0.25 -maxff 20
```
4. *Data transport 1/2.* Like 7., and transport data defined on ‘n10.msh’ to ‘n10-b.msh’. The data are 3D vectors given in file ‘data’ (format = 3 coordinates per line).  

```
$ neper -FM -remesh n10.msh -remeshtess n10.tess -rcl 0.5
  -transport n10.msh 1 elt real3 data -o n10-b
```
5. *Data transport 2/2.* Transport data from an existing old mesh ‘n10.msh’ to an existing new mesh ‘n10-b.msh’. The data are 3D vectors given in file ‘data’ (format = 3 coordinates per line).  

```
$ neper -FM -loadmesh n10-b.msh
  -transport n10.msh 1 elt real3 data -o n10-b
```

## 4 Tessellation Mapped Meshing: `neper -MM`

Module `-MM` is the module to generate a mapped mesh of a tessellation, that is, a mesh comprised of regular, brick elements. Such a mesh does not conform exactly to the tessellation morphology: the interfacial features, and more particularly the grain boundaries and triple lines, have stepped shapes. The input file is a tessellation file (`'tess'`), as provided by module `-T` (in which case the domain must be cuboidal), or simply the data `(n, id)` (same input as for module `-T`, see [Chapter 2 \[Module -T\]](#), page 7). The output mesh can be written in several formats.

In addition to the tessellations generated by module `-T` (or equivalently through the `(n, id)` data), two other types of tessellation can be obtained: *periodic tessellations*, whose grains show periodicity conditions at the domain boundary, and *subdomain-type tessellations*. The latter are cut out from tessellations of larger domains, and which have the same polyhedron volume density. Thus, the tessellations contain grains whose centres are not within the domain. This behaviour is controlled by option `'-ttype'`.

The level of mesh density is specified a bit differently than in module `-FM`. This is done through the following parameter:

- The number of elements along one dimension of the domain (`msize`). For a non-cubic domain, an average, equivalent length of the domain is considered so as to get cubic elements. The number of elements along each of the directions of the domain can also be specified explicitly (option `'-msize3'`).

In the output mesh, the grains are described by element sets. Node sets of the faces, the edges and the vertices of the surface of the tessellation are also provided for prescribing the boundary conditions (option `'-nset'`). The surface element sets (squares) are also provided (option `'-faset'`). The mesh order can be 1 or 2, corresponding to 8-node cubic elements and 20-node cubic elements, respectively (option `'-order'`).

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

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

===== N e p e r =====
Info  : A 3D random polycrystal generator for the finite element method
Info  : Version 1.10.0
Info  : (compiled with: gsl libmatheval)
Info  : Loading initialization file '/home/rquey/.neperrc'...
Info  : -----
Info  : MODULE -MM loaded with arguments:
Info  : [ini file] (none)
Info  : [com line] n10-id1.tess
Info  : -----
Info  : Mapped meshing ...
Info  :   - Loading tessellation ...
Info  :     [i] Parsing file 'n10-id1.tess' ...
Info  :     [i] Parsed file 'n10-id1.tess'.
Info  :   - Generating mesh ...
Info  :     - Searching elsets ... 100%
Info  : Writing results ...
Info  :   - Writing mesh results ...
Info  :     [o] Writing file 'n10-id1.msh' ...
Info  :     [o] Wrote file 'n10-id1.msh'.
```

Info : Elapsed time: 0.033 secs.

=====

## 4.1 Arguments

### 4.1.1 Input Data

The required input data are:

*file\_name* [Input data]  
 Name of the tessellation file.  
 Possible values: **any**. Default value: **none**.

or, the following ones,

**-n integer** [Input data]  
 Number of polyhedra of the tessellation, except for regular morphologies (truncated octahedra, etc., see option '**-morpho**' for details).  
 Possible values: **any**. Default value: **none**.

**-id integer** [Input data]  
 Identifier of the tessellation.  
 Possible values: **any**. Default value: **random**.

**-morpho char\_string** [Input data]  
 Type of morphology of the polyhedra. For random Voronoi tessellations, it can be either equiaxed (**equiaxed**), columnar (**columnar{x,y,z}**) or bamboo-like (**bamboo{x,y,z}**).  
 To load a particular set of polyhedron centres, use the syntax '**@file\_name**' where *file\_name* is the name of a file containing the  $3 * n$  coordinates.  
 Regular morphologies can also be obtained: cubes (**cube**) or truncated octahedra (**tocta**), in which case the value of option '**-n**' stands for the number of polyhedra along an edge of the domain instead of the total number of polyhedra.  
 Possible values: **see above list**. Default value: **equiaxed**.

### 4.1.2 General Options

**-o file\_name** [Option]  
 Specify output file name.  
 Possible values: **any**. Default value: **none**.

### 4.1.3 Domain Options

**-domain char\_string ...** [Option]  
 Specify the type of domain and its size. The only type of domain available is of cuboidal shape (**'cube'**). Then provide the sizes along the x, y and z directions.  
 Possible values: **see above list**. Default value: **cube 1 1 1**.

### 4.1.4 Tessellation Options

This is for a tessellation mesh built from (**n**, **id**) only, not from a tessellation file.

**-scale real real real** [Option]  
 Specify the factors in the x, y and z directions by which the tessellation is to be scaled (once generated).  
 Possible values: **any**. Default value: **none**.

`-ttype char_string` [Option]  
 Specify the type of tessellation (applies to tessellations built with `(n, id)`, not by module `-T` (`.tess` file)). The available values are `'standard'` for a standard tessellation, `periodic` for a periodic tessellation and `subdomain` for a subdomain-type tessellation.  
 Possible values: see above list. Default value: `standard`.

### 4.1.5 Mesh Options

`-msize integer` [Option]  
 Specify the mesh size (number of elements per unit length).  
 Possible values: `any`. Default value: 20.

`-msize3 integer integer integer` [Secondary option]  
 Specify the mesh size (number of elements per unit length) along the x, y and z directions.  
 Possible values: `any`. Default value: 20 20 20.

`-order integer` [Option]  
 Specify the mesh order.  
 Possible values: 1 to 2. Default value: 1.

### 4.1.6 Output Options

`-outdim char_string` [Option]  
 Specify the dimensions of the mesh to output. It can go from 0 to 3, for point to volume elements (combine with commas).  
 Possible values: 0, 1, 2, 3,.. Default value: 3.

`-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. To get the nset corresponding to individual entities, provide their names, that is, for a cubic domain, `[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. Append `'body'` to the name to get only the body nodes of the sets. Combine them with commas.  
 Possible values: `any`. Default value: `faces`.

`-faset char_string` [Option]  
 Specify the domain surfaces to provide. Use `'faces'` for all faces. Combine them with commas.  
 Possible values: `faces`, `[x-z] [0,1]`. Default value: `none`.

## 4.2 Output Files

### 4.2.1 Mesh

The mesh can be written in the following formats:

- Gmsh format: `'msh'`
- Abaqus format: file `'inp'`
- Zset/Zébulon format: `'geof'`

When the input data is of type `(n, id)`, the following file is also generated (as in module `-T`):

- orientation input file: `'oin'`

It contains data for generating the grain orientations, and is an input file for module `-O` (see [Chapter 5 \[Module -O\], page 27](#)).

### 4.3 Examples

Below are some examples of use of neper -MM. Illustrations can be found at [http://neper.sourceforge.net/neper\\_mm.html](http://neper.sourceforge.net/neper_mm.html).

1. Mesh tessellation n100-id1.tess.

```
$ neper -MM n100-id1.tess
```

2. Mesh tessellation n100-id1.tess with 40 elements per unit length.

```
$ neper -MM n100-id1.tess -msize 40
```

3. Provide a mesh of a periodic tessellation made of 100 grains, with identifier 1.

```
$ neper -MM -n 100 -id 1 -msize 40 -ttype periodic
```

## 5 Crystallographic Orientation Generation: neper -O

Module -O is the module to generate crystallographic orientations for the grains of the tessellations generated by module -T. The orientations are randomly distributed according to a uniform distribution. They can be provided according to different descriptors: Euler angles (Bunge, Kocks and Roe conventions), rotation matrix, rotation axis / angle, Rodrigues vector and quaternion. The input data is a file ‘.oin’ provided by module -T (or module -MM), but it can also be the data (n, id). The output data in an orientation file ‘.ori’. Module -O also provides capabilities to generate colours from the orientations (useful for module -VS).

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

```
$ neper -O -n 10 -id 1

===== N e p e r =====
Info  : A 3D random polycrystal generator for the finite element method
Info  : Version 1.10.0
Info  : (compiled with: gsl libmatheval)
Info  : Loading initialization file '/home/rquey/.neperrc'...
Info  : -----
Info  : MODULE -O loaded with arguments:
Info  : [ini file] -crys sym cubic
Info  : [com line] -n 10 -id 1
Info  : -----
Info  :      [o] Writing file 'n10-id1.ori' ...
Info  :      [o] Wrote file 'n10-id1.ori'.
Info  : Elapsed time: 0.001 secs.
=====
```

### 5.1 Arguments

#### 5.1.1 Input Data

The required input data are:

*file.oin* [Input data]

Name of the input file.

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

or, the two following ones:

**-n integer** [Input data]

Number of crystallographic orientations.

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

**-id integer** [Input data]

Identifier of the set of orientations.

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

Alternatively, orientations can be loaded from a file,

**-load input\_type file\_name** [Input data]

Load an orientation file. Provide the type of orientation descriptor (see option ‘-descriptor’) and the file name.

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

### 5.1.2 General Options

**-o *file\_name*** [Option]  
Specify orientation output file name.  
Possible values: **any**. Default value: **none**.

### 5.1.3 Orientation Options

**-crys *char\_string*** [Secondary option]  
Specify the crystal symmetry. This is only used to reduce the domain of definition of the orientation descriptors.  
Possible values: **triclinic** or **cubic**. Default value: **triclinic**.

### 5.1.4 Output Options

**-descriptor *char\_string*** [Option]  
Select the orientation descriptor. It can be Euler angles in Bunge, Kocks or Roe convention (**e**, **ek**, **er**), rotation matrix (**g**), axis / angle or rotation (**rtheta**), Rodrigues vector (**R**) or quaternion (**q**).  
Possible values: **above-mentioned values**. Default value: **e**.

**-format *character\_string*** [Option]  
Specify the format of output file(s). The available formats are: the Neper-native **plain** (i.e. only the descriptors on successive lines), the Zset/Zébulon **geof** and the Fem-Evps **fev** (combine with commas).  
Possible values: **above-mentioned values**. Default value: **plain**.

### 5.1.5 Colouring Options

**-colour *character\_string*** [Option]  
Use this option to get colours from the orientations. Provide as argument the type of colouring: the only one available is from the Rodrigues vectors (**R**). To use this option, **-crys** must be set to **cubic**.  
Possible values: **R**. Default value: **none**.  
Result file: extension **'.col'**.

## 5.2 Output Files

- Crystal orientation file, **'.ori'**: format corresponding to option **'-format'**. The grains orientations are listed on successive lines.
- Orientation colour file, **'.col'**: **red\_level green\_level blue\_level**. The levels are integers comprised in the range [0, 255].

## 5.3 Examples

Below are some examples of use of **neper -O**. Illustrations can be found at [http://neper.sourceforge.net/neper\\_o.html](http://neper.sourceforge.net/neper_o.html).

1. Generate a set of 100 "random" crystallographic orientations, with identifier = 1. Note the uniform distribution.

```
$ neper -O -n 100 -id 1
```

Below are additional examples.

1. *Orientation generation*. Generate a set of crystallographic orientations from the input file **'n100-id1.oin'**.

```
$ neper -O n100-id1.oin
```



2. *Orientation colour generation.* Generate colours which correspond to the orientations written in file 'n100-id1.ori' (Euler angles in Kocks convention).

```
$ neper -O -load ek n100-id1.ori -crys sym cubic -col R
```



## 6 Mesh and Data Visualization: neper -VS

Module -VS is the Neper visualization module, with which the tessellations and meshes can be rendered as publication-quality images. It is also possible to visualize data on them using colours, or displacements of the nodes and to plot data on slices of the mesh. The output file is a PNG image file. Although this module has limited capabilities (compared to visualization applications such as Paraview, etc.), it can be useful for rapid and non-interactive rendering.

Contrary to the other modules, module -VS executes the provided arguments one after the other. Typically, using module -VS consists in loading a tessellation and / or a mesh (options starting by '-load'), then data fields to render them. The data can apply to the tessellation entities: polyhedra, faces, edges and vertices, and to the mesh entities: 3D elements, 2D elements, 1D elements, 0D elements and nodes (options starting by '-data'). The entities that are to be visible on the rendered image, for example particular tessellation polyhedra, element sets or elements, can also be specified (options starting by '-show'). The way they are plotted: camera position and angle, projection type, image size, etc., can be set up as well (options starting by '-camera' or '-image'). The POV-Ray ray-tracing library is used for generating the images.

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

```
$ neper -VS -loadtess n10-id1.tess -loadmesh n10-id1.msh \
        -dataelsetcol ori=n10-id1.ori -print img

===== N e p e r =====
Info  : A 3D random polycrystal generator for the finite element method
Info  : Version 1.10.0
Info  : (compiled with: gsl libmatheval)
Info  : Loading initialization file '/home/rquey/.neperrc'...
Info  : -----
Info  : MODULE -VS loaded with arguments:
Info  : [ini file] -imageantialias 3
Info  : [com line] -loadtess n10-id1.tess -loadmesh n10-id1.msh
Info  : -dataelsetcol ori=n10-id1.ori -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  :   - Reconstructing 2D mesh ... 100%
Info  :   - Reconstructing 1D mesh ... 100%
Info  :   - Reconstructing 0D mesh ... 100%
Info  : Reading data (elset3d, col)...
Info  :   [i] Parsing file 'n10-id1.ori' ...
Info  : Printing image ...
Info  :   [o] Writing file 'img.pov' ...
Info  :   - Printing mesh ...
Info  :     > Preparing mesh data ...
Info  :     > Reducing data ...
Info  :       . Number of 3D elts   reduced by   0% (to 1000).
Info  :       . Number of elt faces reduced by  90% (to 600).
```

```

Info :      . Number of face edges reduced by  0% (to 2400).
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: 0.789 secs.
=====

```

## 6.1 Arguments

### 6.1.1 Tessellation and Mesh Loading

`-loadtess file_name` [Option]  
 Load a tessellation from a file ('.tess').  
 Possible values: **any**. Default value: **none**.

`-loadmesh file_name` [Option]  
 Load a mesh from a file (must be a '.msh').  
 Possible values: **any**. Default value: **none**.

### 6.1.2 Tessellation Data Loading and Rendering

The following options enable to define the properties (colour and size) of the tessellation entities (polyhedra, faces, edges and vertices). This can be done either directly, by specifying the property values (e.g. the RGB channel values for colour) or indirectly, e.g. using scalar values that are rendered in colour using a given *colour 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 image as '`-scaleentity`' as suffix.

`-datapolycol char_string` [Option]  
 Set the colours of the tessellation polyhedra. The argument can be one of the following: the name of a colour that will be used for all polyhedra (see [Appendix C \[Colours\]](#), page 49), the name of a file containing a list of colours (provided as RGB channel values), or a string indicating how the colours can be obtained. The string has the format '`var=file_name`', where '`var`' can be '`ori`' for crystal orientations or '`scal`' for scalar values, and '`file_name`' is the name of the file containing the data. The colour schemes used to derive the colours from the data can be specified with options '`-datapolycolscheme`'.  
 Possible values: **any**. Default value: **white**.

`-datapolycolscheme char_string` [Option]  
 Set the colour scheme used to get colours from the data of the tessellation polyhedra loaded with option '`-datapolycol`'. The type of colour scheme depends on the type of data. For crystal orientations, the colour scheme can be: only "R" for Rodrigues vector colouring; for scalar data, the colour scheme can be any list of colours.  
 Possible values: "R" for crystal orientations and any list of colours for scalars.  
 Default value: "R" for crystal orientations and "blue,cyan,yellow,green" for scalars.

`-datapolyscalemin real` [Option]  
 Set the minimum of the scale relative to the "`-datapolycol scal="` data.  
 Possible values: **any**. Default value: **data minimum**.

- `-datapolyscalemax real` [Option]  
 Set the maximum of the scale relative to the "-datapolycol scal=" data.  
 Possible values: **any**. Default value: **data maximum**.
- `-datapolyscaleticks real` [Option]  
 Set the ticks of the scale relative to the "-datapolycol scal=" data. Provide a string composed of values separated by commas. (Use '\_' to get a blank space.)  
 Possible values: **any**. Default value: **none**.
- `-datafacecol char_string` [Option]  
 Set the colours of the tessellation faces. See option '`-datapolycol`' for the argument format.  
 Possible values: **any**. Default value: **white**.
- `-datafacecolscheme char_string` [Option]  
 Set the colour scheme used to get colours from the data of the tessellation faces loaded with option '`-datafacecol`'. See option '`-datapolycolscheme`' for the argument format.  
 Possible values: **see option '-datapolycolscheme'**. Default value: **see option '-datapolycolscheme'**.
- `-datafacescalemin real` [Option]  
 Set the minimum of the scale relative to the "-datafacecol scal=" data.  
 Possible values: **any**. Default value: **data minimum**.
- `-datafacescalemax real` [Option]  
 Set the maximum of the scale relative to the "-datafacecol scal=" data.  
 Possible values: **any**. Default value: **data maximum**.
- `-datafacescaleticks real` [Option]  
 Set the ticks of the scale relative to the "-datafacecol scal=" data. Provide a string composed of values separated by commas. (Use '\_' to get a blank space.)  
 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 the name of a file containing a list of radii.  
 Possible values: **any**. Default value: **proportional to the polyhedron size**.
- `-dataedgecol char_string` [Option]  
 Set the colours of the tessellation edges. See option '`-datapolycol`' for the argument format.  
 Possible values: **any**. Default value: **black**.
- `-dataedgescheme char_string` [Option]  
 Set the colour scheme used to get colours from the data of the tessellation edges loaded with option '`-dataedgecol`'. See option '`-datapolycolscheme`' for the argument format.  
 Possible values: **see option '-datapolycolscheme'**. Default value: **see option '-datapolycolscheme'**.
- `-dataedgescalemin real` [Option]  
 Set the minimum of the scale relative to the "-dataedgecol scal=" data.  
 Possible values: **any**. Default value: **data minimum**.
- `-dataedgescalemax real` [Option]  
 Set the maximum of the scale relative to the "-dataedgecol scal=" data.  
 Possible values: **any**. Default value: **data maximum**.

- dataedgescaleticks** *real* [Option]  
 Set the ticks of the scale relative to the "-dataedgecol scal=" data. Provide a string composed of values separated by commas. (Use '\_' to get a blank space.)  
 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: **proportional to the polyhedron size**.
- datavercol** *char\_string* [Option]  
 Set the colours of the tessellation vertices. See option '-datapolycol' for the argument format.  
 Possible values: **any**. Default value: **black**.
- datavercolscheme** *char\_string* [Option]  
 Set the colour scheme used to get colours from the data of the tessellation vertices loaded with option '-datavercol'. See option '-datapolycolscheme' for the argument format.  
 Possible values: **see option '-datapolycolscheme'**. Default value: **see option '-datapolycolscheme'**.
- dataverscalemin** *real* [Option]  
 Set the minimum of the scale relative to the "-datavercol scal=" data.  
 Possible values: **any**. Default value: **data minimum**.
- dataverscalemax** *real* [Option]  
 Set the maximum of the scale relative to the "-datavercol scal=" data.  
 Possible values: **any**. Default value: **data maximum**.
- dataverscaleticks** *real* [Option]  
 Set the ticks of the scale relative to the "-datavercol scal=" data. Provide a string composed of values separated by commas. (Use '\_' to get a blank space.)  
 Possible values: **any**. Default value: **none**.

### 6.1.3 Mesh Data Loading and Rendering

The following options enable to define the properties (colour, size, etc.) of the mesh entities (3D, 2D, 1D and 0D elements, nodes). This can be done either directly, by specifying the property values (e.g. the RGB channel values for colour) or indirectly, e.g. using scalar values that are rendered in colour using a given *colour scheme*. In this case, a scale image is generated in addition to the mesh image. The scale properties can be set up (minimum, maximum and tick values). The image as '-scaleentity' as suffix.

The following options enable to load data relative to the 3D mesh elements. Note that **elt3d** can be abbreviated to **elt** in the option names, and that the options can be applied to element sets instead of elements by changing 'elt' to 'elset'.

- dataelt3dcol** *char\_string* [Option]  
 Set the colours of the 3D elements. The argument can be one of the following: the name of a colour that will be used for all elements (see [Appendix C \[Colours\]](#), page 49), the name of a file containing a list of colours (provided as RGB channel values), or a string indicating how the colours can be obtained. The string has the format '**var=file\_name**', where '**var**' can be '**ori**' for crystal orientations or '**scal**' for scalar values, and '**file\_name**' is the name of the file containing the data. The colour schemes used to derive the colours from the data can be specified with options '-dataelt3dcolscheme'.  
 Possible values: **any**. Default value: **white**.

- dataelt3dcolscheme *char\_string*** [Option]  
 Set the colour scheme used to get colours from the data of the 3D elements loaded with option `'-dataelt3dcol'`. The type of colour scheme depends on the type of data. For crystal orientations, the colour scheme can be: only "R" for Rodrigues vector colouring; for scalar data, the colour scheme can be any list of colours.  
 Possible values: "R" for crystal orientations and any list of colours for scalars.  
 Default value: "R" for crystal orientations and "blue,cyan,yellow,green" for scalars.
- dataelt3dscalemin *real*** [Option]  
 Set the minimum of the scale relative to the `"-dataelt3dcol scal="` data.  
 Possible values: any. Default value: data minimum.
- dataelt3dscalemax *real*** [Option]  
 Set the maximum of the scale relative to the `"-dataelt3dcol scal="` data.  
 Possible values: any. Default value: data maximum.
- dataelt3dscaleticks *real*** [Option]  
 Set the ticks of the scale relative to the `"-dataelt3dcol scal="` data. Provide a string composed of values separated by commas. (Use `'_'` to get a blank space.)  
 Possible values: any. Default value: none.
- dataelt3dedgecol *char\_string*** [Option]  
 Set the colours of the edges of the 3D elements. See option `'-dataelt3dcol'` for the argument format.  
 Possible values: any. Default value: black.
- dataelt3dedgecolscheme *char\_string*** [Option]  
 Set the colour scheme used to get colours from the data of the element edges loaded with option `'-dataelt3dedgecol'`. See option `'-dataelt3dcolscheme'` for the argument format.  
 Possible values: see option `'-dataelt3dcolscheme'`. Default value: see option `'-dataelt3dcolscheme'`.
- dataelt3dedgerad *char\_string*** [Option]  
 Set the radii of the edges of the 3D elements. The argument can be one of the following: a real value that will be used for all entities, or the name of a file containing a list of radii.  
 Possible values: any. Default value: proportional to the polyhedron size.

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

- dataelt2dcol *char\_string*** [Option]  
 Set the colours of the 2D elements. See option `'-dataelt3dcol'` for the argument format.  
 Possible values: any. Default value: black.
- dataelt2dcolscheme *char\_string*** [Option]  
 Set the colour scheme used to get colours 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'`.
- dataelt2dscalemin *real*** [Option]  
 Set the minimum of the scale relative to the `"-dataelt2dcol scal="` data.  
 Possible values: any. Default value: data minimum.

`-dataelt2dscalemax` *real* [Option]

Set the maximum of the scale relative to the "-dataelt2dcol scal=" data.

Possible values: **any**. Default value: **data maximum**.

`-dataelt2dscaleticks` *real* [Option]

Set the ticks of the scale relative to the "-dataelt2dcol scal=" data. Provide a string composed of values separated by commas. (Use '\_' to get a blank space.)

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

`-dataelt2dedgecol` *char\_string* [Option]

Set the colours of the edges of the 3D elements. See option '`-dataelt3dcol`' for the argument format.

Possible values: **any**. Default value: **black**.

`-dataelt2dedgecolscheme` *char\_string* [Option]

Set the colour scheme used to get colours from the data of the edges of the 2D elements loaded with option '`-dataelt2dedgecol`'. See option '`-dataelt3dcolscheme`' for the argument format.

Possible values: see option '`-dataelt3dcolscheme`'. Default value: see option '`-dataelt3dcolscheme`'.

`-dataelt2dedgescalemin` *real* [Option]

Set the minimum of the scale relative to the "-dataelt2dedgecol scal=" data.

Possible values: **any**. Default value: **data minimum**.

`-dataelt2dedgescalemax` *real* [Option]

Set the maximum of the scale relative to the "-dataelt2dedgecol scal=" data.

Possible values: **any**. Default value: **data maximum**.

`-dataelt2dedgescaleticks` *real* [Option]

Set the ticks of the scale relative to the "-dataelt2dedgecol scal=" data. Provide a string composed of values separated by commas. (Use '\_' to get a blank space.)

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

`-dataelt2dedgerad` *char\_string* [Option]

Set the radii of the edges of the 3D elements. The argument can be one of the following: a real value that will be used for all entities, or the name of a file containing a list of radii.

Possible values: **any**. Default value: **proportional to the polyhedron size**.

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

`-dataelt1dcol` *char\_string* [Option]

Set the colours of the 1D elements. See option '`-dataelt3dcol`' for the argument format.

Possible values: **any**. Default value: **black**.

`-dataelt1dcolscheme` *char\_string* [Option]

Set the colour scheme used to get colours 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`'.

`-dataelt1dscalemin` *real* [Option]

Set the minimum of the scale relative to the "-dataelt1dcol scal=" data.

Possible values: **any**. Default value: **data minimum**.



`-dataelt1dscalemax` *real* [Option]

Set the maximum of the scale relative to the "-dataelt1dcol scal=" data.

Possible values: **any**. Default value: **data maximum**.

`-dataelt1dscaleticks` *real* [Option]

Set the ticks of the scale relative to the "-dataelt1dcol scal=" data. Provide a string composed of values separated by commas. (Use '\_' to get a blank space.)

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

`-dataelt1drad` *char\_string* [Option]

Set the radii of the 1D element. See option '`-dataelt3dedgerad`' for the argument format.

Possible values: **any**. Default value: **proportional to 3D elset size**.

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

`-dataelt0dcol` *char\_string* [Option]

Set the colours of the 0D elements. See option '`-dataelt3dcol`' for the argument format.

Possible values: **any**. Default value: **black**.

`-dataelt0dcolscheme` *char\_string* [Option]

Set the colour scheme used to get colours 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`'**.

`-dataelt0dscalemin` *real* [Option]

Set the minimum of the scale relative to the "-dataelt0dcol scal=" data.

Possible values: **any**. Default value: **data minimum**.

`-dataelt0dscalemax` *real* [Option]

Set the maximum of the scale relative to the "-dataelt0dcol scal=" data.

Possible values: **any**. Default value: **data maximum**.

`-dataelt0dscaleticks` *real* [Option]

Set the ticks of the scale relative to the "-dataelt0dcol scal=" data. Provide a string composed of values separated by commas. (Use '\_' to get a blank space.)

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

`-dataelt0drad` *char\_string* [Option]

Set the radii of the 0D element. See option '`-dataelt3dedgerad`' for the argument format.

Possible values: **any**. Default value: **proportional to 3D elset size**.

The following options enable to load data relative to the nodes.

`-datanodecoo` *char\_string* [Option]

Set the coordinates of the nodes. The argument can be the name of a file containing a list of coordinates, or a string indicating how the coordinates can be obtained. The string has the format '`var=file_name`', where '`var`' can be '`disp`' for displacements, and '`file_name`' is the name of the file containing the data.

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**.

- `-datanodecol file_name` [Option]  
 Set the colours of the nodes. See option '`-dataelt3dcol`' for the argument format.  
 Possible values: **any**. Default value: **black**.
- `-datanodecolscheme char_string` [Option]  
 Set the colour scheme used to get colours 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`'**.
- `-datanodescalemin real` [Option]  
 Set the minimum of the scale relative to the "`-datanodecol scal="` data.  
 Possible values: **any**. Default value: **data minimum**.
- `-datanodescalemax real` [Option]  
 Set the maximum of the scale relative to the "`-datanodecol scal="` data.  
 Possible values: **any**. Default value: **data maximum**.
- `-datanodescaleticks real` [Option]  
 Set the ticks of the scale relative to the "`-datanodecol scal="` data. Provide a string composed of values separated by commas. (Use '`_`' to get a blank space.)  
 Possible values: **any**. Default value: **none**.
- `-datanoderad file_name` [Option]  
 Set the radii of the nodes. See option '`-dataeltedgerad`' for the argument format.  
 Possible values: **any**. Default value: **none**.

The following options enable to colour the elements from data defined at the nodes.

- `-datanode2eltcol file_name` [Option]  
 Set the colours of the elements from values defined at the nodes. See option '`-dataelt3dcol`' for the argument format.  
 Possible values: **any**. Default value: **black**.
- `-datanode2eltcolscheme char_string` [Option]  
 Set the colour scheme used to get colours from the data loaded with option '`-datanode2eltcol`'. See option '`-dataelt3dcolscheme`' for the argument format.  
 Possible values: **see option '`-dataelt3dcolscheme`'**. Default value: **see option '`-dataelt3dcolscheme`'**.
- `-datanode2eltscalemin real` [Option]  
 Set the minimum of the scale relative to the "`-datanode2eltcol scal="` data.  
 Possible values: **any**. Default value: **data minimum**.
- `-datanode2eltscalemax real` [Option]  
 Set the maximum of the scale relative to the "`-datanode2eltcol scal="` data.  
 Possible values: **any**. Default value: **data maximum**.
- `-datanode2eltscaleticks real` [Option]  
 Set the ticks of the scale relative to the "`-datanode2eltcol scal="` data. Provide a string composed of values separated by commas. (Use '`_`' to get a blank space.)  
 Possible values: **any**. Default value: **none**.

### 6.1.4 Slice Settings

**-slicemesh *char\_string*** [Option]  
 Use this option to plot one (or several) slice(s) of the mesh. Provide as argument the equation of the plane, under the form  $\{x,y,z\}=value$  (combine with commas). This option works for free meshes only (tetrahedral elements).  
 Possible values: **any**. Default value: **none**.

### 6.1.5 Show Settings

The following options apply to the full tessellation or mesh.

**-showtess *logical*** [Option]  
 Use this option to show or hide the tessellation.  
 Possible values: 0 or 1. Default value: 1 if tess loaded and no mesh.

**-showmesh *logical*** [Option]  
 Use this option to show or hide the mesh.  
 Possible values: 0 or 1. Default value: 1 if mesh loaded and no slice.

The following options apply to the entities of the tessellation.

**-showpoly *char\_string*** [Option]  
 Specify the polyhedra to show. The argument can be: 'all' for all, '*file\_name*' to load polyhedron identifiers from a file, or any expression based on the following arguments: *id*, *cenx*, *ceny*, *cenz*, *volume*, *true*, *body*, and *faceqty*.  
 Possible values: **any**. Default value: **all** if tess loaded.

**-showface *char\_string*** [Option]  
 Specify the faces to show. The argument can be: 'all' for all, '*@file\_name*' to load face identifiers from a file, or any expression based on the following arguments: *id*, *cenx*, *ceny*, *cenz*, *area*, *ff*, *true*, *body*, *verqty*, *edgeqty* 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, '*@file\_name*' to load edge numbers from a file, or any expression based on the following arguments: *id*, *cenx*, *ceny*, *cenz*, *length*, *true*, *body*, *face-shown*, *poly-shown* and *cyl*. The *cyl* variable is useful to hide "fake" edges which would appear within the faces of the grains which are on the circular part of a cylinder. Use argument *cyl==0* to hide them.  
 Possible values: **any**. Default value: **none**.

**-showver *char\_string*** [Option]  
 Specify the vertices to show. The argument can be: 'all' for all, '*@file\_name*' to load vertex numbers from a file, or any expression based on the following arguments: *id*, *cenx*, *ceny*, *cenz*, *true*, *body*, *edge-shown*, *face-shown* and *poly-shown*.  
 Possible values: **any**. Default value: **none**.

**-showfaceinter *logical*** [Secondary option]  
 Show the interpolations of the tessellation faces (if any).  
 Possible values: 0 or 1. Default value: 0.

The following options apply to the entities of the mesh.

- showelt *char\_string*** [Option]  
 Specify the elements to show. The argument can be: ‘all’ for all , ‘@*file\_name*’ to load element numbers from a file, or any expression based on the following arguments: *id*, *cenx*, *ceny*, *cenz*, *volume*, *elset\_true*, *elset\_body* and *elset\_id*.  
 Possible values: any. Default value: all if mesh loaded (and no tessellation) and nothing -show’d.
- showelset *char\_string*** [Option]  
 Specify element sets to show. Refer to option ‘-showpoly’ for the available arguments.  
 Possible values: any. Default value: none.
- showeltid *char\_string*** [Option]  
 Specify the 1D elements to show. The argument can be: ‘all’ for all , ‘@*file\_name*’ to load element numbers from a file, or any expression based on the following arguments: *cenx*, *ceny*, *cenz*, *length*, *elset\_true*, *elset\_body*, *id*, *elt3d\_shown* and *cyl*. The *cyl* variable is useful to hide “fake” 1-D elements which would appear within the faces of the grains which are on the circular part of a cylinder. Use argument *cyl*==0 to hide them.  
 Possible values: any. Default value: none.
- showshadow *logical*** [Option]  
 Show the shadows. If you want “true” colours, switch this option off.  
 Possible values: 0 or 1. Default value: 1.

### 6.1.6 Camera Settings

- cameracoo[,*x,y,z*] *char\_string*** [Option]  
 Specify the camera coordinates. The expression can be based on the following arguments: *tesscentre*, *meshcentre*, *v* and *cameralookat*.  
 Possible values: any. Default value: *cameralookat+v*.
- cameralookat[,*x,y,z*] *char\_string*** [Option]  
 Specify the point the camera looks at. The expression can be based on the following arguments: *O* (the origin), *tesscentre* and *meshcentre*.  
 Possible values: any. Default value: *tesscentre* if *tess* printed, *meshcentre* if *mesh* printed.
- cameraangle *real*** [Option]  
 Specify the opening angle of the camera along the horizontal direction (degrees).  
 Possible values: any. Default value: 25.
- cameraprojection *char\_string*** [Option]  
 Specify the type of projection of the camera.  
 Possible values: *perspective* or *orthographic*. Default value: *perspective*.

### 6.1.7 Output Image Settings

- imagesize *integer integer*** [Option]  
 Specify the width and height of the image (in pixels).  
 Possible values: any any. Default value: 1200 900.
- imagebackground *real real real*** [Option]  
 Specify the colour of the background (normed RGB levels).  
 Possible values: any. Default value: 1 1 1.
- imageantialias *integer*** [Option]  
 Use antialiasing to produce a smoother image.  
 Possible values: any (consider 1 to 3). Default value: 0.

**-imageformat *string*** [Option]  
 Specify the format of the output image.  
 Possible values: **png** or **pov**. Default value: **png**.

### 6.1.8 Scripting

**-loop *char\_string* *real* *real* *real* ... -endloop** [Option]  
 Use this option to make a loop. Provide as argument the name of the loop variable, its initial value, the loop increment value, the final value, then 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**.

### 6.1.9 Advanced Options

**-includepov *char\_string*** [Option]  
 Use this option to include additional objects to the figure, under the form of a POV-Ray file. Provide as argument the name of the POV-Ray file.  
 Possible values: **any**. Default value: **none**.

## 6.2 Output Files

The output files are:

- Image file, '**.png**': a bitmapped image (the alpha channel is off).
- POV-Ray file, '**.pov**': a POV-Ray script file.

A PNG image can be obtained from the '**.pov**' file by invoking POV-Ray as follows (see the POV-Ray documentation for details and further commands):

```
$ povray Input_File_Name=file.pov +Wimage_width +Himage_height -D .
```

## 6.3 Examples

Below are some examples of use of neper -VS. Illustrations can be found at [http://neper.sourceforge.net/neper\\_vs.html](http://neper.sourceforge.net/neper_vs.html).

1. Print out tessellation n100-id1.tess as image 'img.png'.  

```
$ neper -VS -loadtess n100-id1.tess -print img
```
2. Print out tessellation n100-id1.tess with a camera angle of 12 degrees, an image size of 400x400 pixels and an image antialiasing level of 2 (better quality).  

```
$ neper -VS -loadtess n100-id1.tess -cameraangle 12 -imagesize 400  
400 -imageantialias 2 -print img
```
3. Print out tessellation n100-id1.tess with the colours written in file 'n100-id1.col' to render the grains.  

```
$ neper -VS -loadtess n100-id1.tess -datapolycol n100-id1.col  
-cameraangle 12 -imagesize 400 400 -imageantialias 2 -print img
```
4. Print out tessellation n100-id1.tess with the colours written in file 'n100-id1.col' to render the grains and nicely shown vertices and edges.  

```
$ neper -VS -loadtess n100-id1.tess -datapolycol n100-id1.col  
-dataverrad 0.03 -dataedgerad 0.015 -datavercol red -dataedgecol  
0:90:180 -cameraangle 12 -imagesize 400 400 -imageantialias 2  
-print img
```

5. Print out tessellation n100-id1.tess with the grains coloured according to their orientations (orientation file: 'n100-id1.ori').

```
$ neper -VS -loadtess n100-id1.tess -datapolycol
ori=n100-id1.ori -cameraangle 12 -imagesize 400 400
-imageantialias 2 -print img
```

6. Print out mesh n100-id1.msh as image 'img.png'. Set the radius of the element edges to 0.0015 and the radius of the 1D element edges to 0.0045.

```
$ neper -VS -loadmesh n100-id1.msh -dataeltdgerad 0.0015
-dataelt1drad 0.0045 -cameraangle 12 -imagesize 400 400
-imageantialias 2 -print img
```

7. Print out mesh n100-id1.msh with the colours written in file 'n100-id1.col' to render the grains.

```
$ neper -VS -loadmesh n100-id1.msh -dataelsetcol
ori=n100-id1.ori -dataeltdgerad 0.0015 -dataelt1drad 0.0045
-cameraangle 12 -imagesize 400 400 -imageantialias 2 -print img
```

8. Print out mesh n100-id1.msh, but only the inner grains.

```
$ neper -VS -loadmesh n100-id1.msh -dataelsetcol ori=n100-id1.ori
-showelset "body>0" -dataeltdgerad 0.0015 -dataelt1drad 0.0045
-cameraangle 12 -imagesize 400 400 -imageantialias 2 -print img
```

9. Print out mesh n100-id1.msh, but only the elements with  $z < 0.5$ .

```
$ neper -VS -loadmesh n100-id1.msh -dataelsetcol ori=n100-id1.ori
-showelt "cenz<0.5" -dataeltdgerad 0.0015 -dataelt1drad 0.0045
-cameraangle 12 -imagesize 400 400 -imageantialias 2 -print img
```

10. Print out 3 slices of mesh n100-id1.msh.

```
$ neper -VS -loadmesh n100-id1.msh -dataelsetcol ori=n100-id1.ori
-slicemesh "x=0.5,y=0.5,z=0.5" -cameraangle 12 -imagesize 400
400 -imageantialias 2 -print img
```

## Appendix A File Formats

### A.1 Tessellation file ‘.tess’

Here are details on the ‘.tess’ file format version 1.10. The developers may note that read and write functions are available as `neut_geo_fscanf()` and `neut_geo_fprintf()`, defined in directories ‘neut/neut\_geo/neut\_geo\_fscanf’ and ‘neut/neut\_geo/neut\_geo\_fprintf’.

```
***tess
**format
    format
**general
    n id type morphology
**vertex
    total_number_of_vertices
    ver_id  dom_entity_type dom_entity_id
           number_of_edges edge_1 edge_2 ...
           ver_x ver_y ver_z ver_state
    ...
**edge
    total_number_of_edges
    edge_id dom_entity_type dom_entity_id
           ver_1 ver_2
           number_of_faces face_1 face_2 ...
           edge_state
    ...
**face
    total_number_of_faces
    face_id dom_entity_type dom_entity_id
           poly_1 poly_2
           face_eq_a face_eq_b face_eq_c face_eq_d
           number_of_vertices ver_1 ver_2 ...
                               edge_1* edge_2* ... (As many edges as vertices.)
           face_state face_point face_point_x face_point_y face_point_z
           face_ff
    ...
**polyhedron
    total_number_of_polyhedra
    poly_id poly_centre_x poly_centre_y poly_centre_z
           poly_true poly_body
           number_of_faces face_1* face_2* ...
    ...
**domain
    *general
        dom_type
    *vertex
        total_number_of_dom_vertices
        dom_ver_id ver_1
                number_of_edges dom_edge_1 dom_edge_2 ...
    ...
    *edge
```

```

total_number_of_dom_edges
dom_edge_id number_of_dom_tess_edges edge_1 edge_2 ...
            dom_ver_1 dom_ver_2
            dom_face_1 dom_face_2
...
*face
total_number_of_dom_faces
dom_face_id number_of_dom_tess_faces dom_tess_face_1 dom_tess_face_2 ...
            dom_face_eq_a dom_face_eq_b dom_face_eq_c dom_face_eq_d
            number_of_dom_vertices dom_ver_1 dom_ver_2 ...
                                   dom_edge_1 dom_edge_2 ...
...
***end

```

where (with identifiers being integer numbers)

- *format* is the file format, currently '1.10' (character string).
- *n* is the number of polyhedra of the tessellation (option '-n').
- *id* is the identifier of the tessellation (option '-id').
- *type* is the type of tessellation (always 'standard').
- *morphology* is a character string indicating the morphology of the tessellation or polyhedra (option '-morpho'). It equals to 'poisson' for a Poisson Voronoi tessellation, 'tocta' for truncated octahedra, 'columnar[x,y,z]' for columnar grains, 'bamboo[x,y,z]' for bamboo grains or 'custom' for user-specified coordinates of the polyhedron germs (use of option '-centrecoo').
- *total\_number\_of\_vertices* is the total number of vertices.
- *dom\_entity\_type* is an integer equal to the type of domain entity that a tessellation vertex, edge or face belongs to. The value is equal to 0 for a domain vertex, 1 for a domain edge and 2 for a domain face, and -1 for none.
- *dom\_entity\_id* is the identifier of a domain entity that a tessellation vertex, edge or face belongs to. The domain entity can be a domain vertex, edge or face, as indicated by *dom\_entity\_type*. If *dom\_entity\_type* = -1, *dom\_entity\_id* carries on no information and has a value of 0.
- *ver\_id* is the identifier of a vertex and ranges from 1 to *total\_number\_of\_vertices*.
- *number\_of\_edges* is the number of edges a vertex belongs to.
- *edge\_1*, *edge\_2*, ... are identifiers of edges.
- *edge\_1\**, *edge\_2\**, ... are identifiers of the edges of a face, signed according to their orientation in the face.
- *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.
- *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.
- *number\_of\_faces* is the number of faces an edge belongs to, or to the number of faces a polyhedron has, depending on the context.
- *face\_1*, *face\_2*, ... are identifiers of faces.



- *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).
- *edge\_state* is an integer indicating the state of an edge (always 0).
- *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*.
- *poly\_1* and *poly\_2* are identifiers of polyhedra. *poly2* is negative if the face belongs to a domain face, thereby having only one parent polyhedron. In that case, its value is negative *dom\_entity\_id*.
- *face\_eq\_a*, *face\_eq\_b*, *face\_eq\_c* and *face\_eq\_d* are the parameters of the equation of a face:  $\text{face\_eq\_a}x + \text{face\_eq\_b}y + \text{face\_eq\_c}z = \text{face\_eq\_d}$ . The parameters are scaled so that  $\text{face\_eq\_a}^2 + \text{face\_eq\_b}^2 + \text{face\_eq\_c}^2 = 1$ .
- *number\_of\_vertices* is the number of vertices that a face has.
- *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 (the list being: *ver\_1 ver\_2 ...*). 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).
- *face\_ff* is a real value equal to the “flatness fault” of a face. For a standard tessellation, it equals 0. For a regularized tessellation, it is the maximum angle between the normals at two points of a face, expressed in degrees.
- *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*.
- *poly\_centre\_x*, *poly\_centre\_y* and *poly\_centre\_z* are the coordinates of the centre of a polyhedron.
- *poly\_true* is an integer equal to the “true” value of a polyhedron (see [Chapter 3 \[Module -FM\], page 13](#)).
- *poly\_body* is an integer equal to the “body” value of a polyhedron (see [Chapter 3 \[Module -FM\], page 13](#)).
- *dom\_type* is the type of the domain (one of *cube*, *cylinder*, *poly* and *planes*).
- *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*.
- *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\_tess\_edges* is the number of tessellation edges that a domain edge has.
- *dom\_ver\_1*, *dom\_ver\_2*, ... are identifiers of the domain vertices that a domain edge or face has.
- *dom\_face\_1* and *dom\_face\_2* are identifiers of the domain faces that a domain edge has.
- *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\_tess\_faces* is the number of tessellation faces that a domain face has.
- *dom\_tess\_face\_1*, *dom\_tess\_face\_2*, ... are the identifiers of the tessellation faces that a domain face has.
- *dom\_face\_eq\_a*, *dom\_face\_eq\_b*, *dom\_face\_eq\_c* and *dom\_face\_eq\_d* are the parameters of the equation of a domain face and are defined in the same way than *face\_eq\_a*, etc. (see above).
- *number\_of\_dom\_vertices* is the number of domain vertices (and edges) that a domain face has.
- *dom\_edge\_1*, *dom\_edge\_2*, ... are identifiers of the domain edges that a domain face has.

## Appendix B Mathematical and Logical Expressions

### B.1 Mathematical Expressions

Neper can handle mathematical expressions. It makes use of the GNU `libmatheval` library. The expression must contain no space, tabulation or new-line characters, and match the following syntax<sup>1</sup>:

Supported constants are (names that should be used are given in parenthesis): `e` (`e`), `log2(e)` (`log2e`), `log10(e)` (`log10e`), `ln(2)` (`ln2`), `ln(10)` (`ln10`), `pi` (`pi`), `pi / 2` (`pi_2`), `pi / 4` (`pi_4`), `1 / pi` (`1_pi`), `2 / pi` (`2_pi`), `2 / sqrt(pi)` (`2_sqrtpi`), `sqrt(2)` (`sqrt`) and `sqrt(1 / 2)` (`sqrt1_2`).

Variable name is any combination of alphanumericals and `_` characters beginning with a non-digit that is not elementary function name.

Supported elementary functions are (names that should be used are given in parenthesis): exponential (`exp`), logarithmic (`log`), square root (`sqrt`), sine (`sin`), cosine (`cos`), tangent (`tan`), cotangent (`cot`), secant (`sec`), cosecant (`csc`), inverse sine (`asin`), inverse cosine (`acos`), inverse tangent (`atan`), inverse cotangent (`acot`), inverse secant (`asec`), inverse cosecant (`acsc`), hyperbolic sine (`sinh`), cosine (`cosh`), hyperbolic tangent (`tanh`), hyperbolic cotangent (`coth`), hyperbolic secant (`sech`), hyperbolic cosecant (`csch`), hyperbolic inverse sine (`asinh`), hyperbolic inverse cosine (`acosh`), hyperbolic inverse tangent (`atanh`), hyperbolic inverse cotangent (`acoth`), hyperbolic inverse secant (`asech`), hyperbolic inverse cosecant (`acsch`), absolute value (`abs`), Heaviside step function (`step`) with value 1 defined for  $x = 0$ , Dirac delta function with infinity (`delta`) and not-a-number (`nandelta`) values defined for  $x = 0$ , and error function (`erf`).

Supported unary operation is unary minus (`'-'`).

Supported binary operations are addition (`'+'`), subtraction (`'-'`), multiplication (`'*'`), division (`'/'`) and exponentiation (`'^'`).

Usual mathematical rules regarding operation precedence apply. Parenthesis (`'('` and `')'`) could be used to change priority order.

Neper includes additional functions: the minimum function (`min(a,b)`) and the maximum function (`max(a,b)`). `a` and `b` can be any expression following the above-described syntax. Moreover, square brackets (`'['` and `']'`) and curly brackets (`'{'` and `'}'`) can be used instead of the parentheses.

### B.2 Logical Expressions

The logical operators supported are: `=` (`==`), `≠` (`!=`), `≥` (`>=`), `≤` (`<=`), `>` (`>`), `<` (`<`), AND (`&&`) and OR (`||`).

---

<sup>1</sup> Taken from the `libmatheval` documentation.



## Appendix C Colours

Colours can be specified in two ways: by name or by RGB channel values, as detailed in the following.

Here is the list of the available colours (character string and RGB channel values):

aliceblue (240, 248, 255), antiquewhite (250, 235, 215), aqua (0, 255, 255), aquamarine (127, 255, 212), azure (240, 255, 255), beige (245, 245, 220), bisque (255, 228, 196), black (0, 0, 0), blanchedalmond (255, 235, 205), blue (0, 0, 255), blueviolet (138, 43, 226), brown (165, 42, 42), burlywood (222, 184, 135), cadetblue (95, 158, 160), chartreuse (127, 255, 0), chocolate (210, 105, 30), coral (255, 127, 80), cornflowerblue (100, 149, 237), cornsilk (255, 248, 220), crimson (220, 20, 60), cyan (0, 255, 255), darkblue (0, 0, 139), darkcyan (0, 139, 139), darkgoldenrod (184, 134, 11), darkgray (64, 64, 64), darkgreen (0, 100, 0), darkgrey (64, 64, 64), darkkhaki (189, 183, 107), darkmagenta (139, 0, 139), darkolivegreen (85, 107, 47), darkorange (255, 140, 0), darkorchid (153, 50, 204), darkred (139, 0, 0), darksalmon (233, 150, 122), darkseagreen (143, 188, 143), darkslateblue (72, 61, 139), darkslategray (47, 79, 79), darkslategrey (47, 79, 79), darkturquoise (0, 206, 209), darkviolet (148, 0, 211), deeppink (255, 20, 147), deepskyblue (0, 191, 255), dimgray (105, 105, 105), dimgrey (105, 105, 105), dodgerblue (30, 144, 255), firebrick (178, 34, 34), floralwhite (255, 250, 240), forestgreen (34, 139, 34), fuchsia (255, 0, 255), gainsboro (220, 220, 220), ghostwhite (248, 248, 255), gold (255, 215, 0), goldenrod (218, 165, 32), gray (128, 128, 128), grey (128, 128, 128), green (0, 255, 0), greenyellow (173, 255, 47), honeydew (240, 255, 240), hotpink (255, 105, 180), indianred (205, 92, 92), indigo (75, 0, 130), ivory (255, 255, 240), khaki (240, 230, 140), lavender (230, 230, 250), lavenderblush (255, 240, 245), lawngreen (124, 252, 0), lemonchiffon (255, 250, 205), lightblue (173, 216, 230), lightcoral (240, 128, 128), lightcyan (224, 255, 255), lightgoldenrodyellow (250, 250, 210), lightgray (211, 211, 211), lightgreen (144, 238, 144), lightgrey (211, 211, 211), lightpink (255, 182, 193), lightsalmon (255, 160, 122), lightseagreen (32, 178, 170), lightskyblue (135, 206, 250), lightslategray (119, 136, 153), lightslategrey (119, 136, 153), lightsteelblue (176, 196, 222), lightyellow (255, 255, 224), lime (0, 255, 0), limegreen (50, 205, 50), linen (250, 240, 230), magenta (255, 0, 255), maroon (128, 0, 0), mediumaquamarine (102, 205, 170), mediumblue (0, 0, 205), mediumorchid (186, 85, 211), mediumpurple (147, 112, 219), mediumseagreen (60, 179, 113), mediumslateblue (123, 104, 238), mediumspringgreen (0, 250, 154), mediumturquoise (72, 209, 204), mediumvioletred (199, 21, 133), midnightblue (25, 25, 112), mintcream (245, 255, 250), mistyrose (255, 228, 225), moccasin (255, 228, 181), navajowhite (255, 222, 173), navy (0, 0, 128), oldlace (253, 245, 230), olive (128, 128, 0), olivedrab (107, 142, 35), orange (255, 165, 0), orangered (255, 69, 0), orchid (218, 112, 214), palegoldenrod (238, 232, 170), palegreen (152, 251, 152), paleturquoise (175, 238, 238), palevioletred (219, 112, 147), papayawhip (255, 239, 213), peachpuff (255, 218, 185), peru (205, 133, 63), pink (255, 192, 203), plum (221, 160, 221), powderblue (176, 224, 230), purple (128, 0, 128), red (255, 0, 0), rosybrown (188, 143, 143), royalblue (65, 105, 225), saddlebrown (139, 69, 19), salmon (250, 128, 114), sandybrown (244, 164, 96), seagreen (46, 139, 87), seashell (255, 245, 238), sienna (160, 82, 45), silver (192, 192, 192), skyblue (135, 206, 235), slateblue (106, 90, 205), slategray (112, 128, 144), slategrey (112, 128, 144), snow (255, 250, 250), springgreen (0, 255, 127), steelblue (70, 130, 180), tan (210, 180, 140), teal (0, 128, 128), thistle (216, 191, 216), tomato (255, 99, 71), turquoise (64, 224, 208), violet (238, 130, 238), wheat (245, 222, 179), white (255, 255, 255), whitesmoke (245, 245, 245), yellow (255, 255, 0), yellowgreen (154, 205, 50).

Any other colour of known RGB channel values can be defined by forming a character string of format: ‘R\_value,G\_value,B\_value’. The ‘,’ separator can be changed to one of ‘/’, ‘.’, ‘:’ and ‘;’.



## Appendix D Versions

New in 1.10.0 (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 (September 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  $\geq 2.4.2$ ). Strongly reduced memory usage.
- 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 *-euleranglesconvention* (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

GNU General Public License

Version 3, 29 June 2007

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