Neper Reference Manual

The documentation for Neper 1.9.2
A 3D random polycrystal generator for the finite element method

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- *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 1.9),* `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, and can be deformed to account for morphological texture.
- Module -FM aims at generating free 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 simultaneous use of several meshers), and remeshing.
- Module -MM is for generating mapped meshes of tessellations. These meshes are comprised of regular, brick-shape elements, and 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 capabilities of Neper 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 a brief introduction to Neper, as well as examples of use and illustrations (images and videos).
- 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`.

1.2 Installing Neper

1.2.1 Dependencies

Neper is written in C and can be compiled and run under any Unix-like system. You will need a C compiler (e.g. the GNU compiler `gcc`). Neper has several dependencies, which may be mandatory or optional. The optional libraries enable some advanced capabilities. The dependencies 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`, and installed by following the instructions provided in the reference manual.

- the Gmsh program (not needed at compilation, but 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 (not needed at compilation, but 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`.

- the libmatheval library (optional)

  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`, and installed by following the instructions provided in the reference manual. By default, Neper is compiled *with* libmatheval support.

- the libScotch library (optional)

  Module -FM includes mesh partitioning capabilities, which make use of the Scotch mesh partitioner (version `5.1.10` or later). It can be downloaded from the Scotch homepage, `www.labri.fr/perso/pelegrin/scotch`, and installed by following the instructions provided in the reference manual. By default, Neper is compiled *without* libScotch support.

Whether or not Neper is to be compiled with support of one of the optional libraries can be indicated in file '`dependencies.h`', through the macros `HAVE_`*`LIBRARYNAME`*. Their values have to be set to '`1`' if the library is to be supported and '`0`' otherwise. The '`Makefile`' file must also be modified: linking information for the libraries may have to be added to the *LINKFLAGS* variable, as detailed in the '`Makefile`' file. After modifying the '`dependencies.h`' file, make sure to clean up the project through the command `make clean` before compiling.

1.2.2 Installation

Neper can be compiled as follows:

```
$ make;
```

and

```
$ make install;
```

to copy the binary file to the standard system location ('`/usr/local/bin/`').

Moreover, the documentation can be installed as an '`info`' file. On most systems, this can be achieved simply by copying the file '`neper.info`' into an info directory (usually '`/usr/info`', '`/usr/local/info`' or '`/usr/doc/info`').

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.

1.4 Acknowledgments

Neper is a long-winded project which has been carried on by Romain Quey since 2003, while he was at INSA de Rouen (France), Cornell University (USA) and the École Nationale Supérieure des Mines de Saint-Étienne (France). Christophe Geuzaine and François Pelegrinni are acknowledged for the help they have provided regarding the integration of the Gmsh and libScotch libraries, respectively.

2 Tessellation Generation: neper -T

Module -T enables one to generate Voronoi tessellations of a space *domain* of any brick 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, arrangment of polyhedra (truncated octahedra are currently available). Another capability is 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 exhasutively the polycrystal morphology, The '`.tess`' file is an input file of the meshing modules, -FM and -MM (see Chapter 3 [Module -FM], page 11 and Chapter 4 [Module -MM], page 21). Module -T also generates as output a '`.oin`' file, which contains input data for the crystallographic orientation generation (see Chapter 5 [Module -O], page 25). The generated tessellation ('`.tess`' file) can be visualized with module -VS (Chapter 6 [Module -VS], page 29).

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 1.9.2 (18 Sept 2011)
Info   : (compiled with: gsl, libmatheval, libscotch)
Info   : Loading initialization file '/home/rquey/.neperrc'...
Info   : ---------------------------------------------------------------
Info   : MODULE  -T run with arguments:
Info   : [ini file]
Info   : [com line] -n 10 -id 1
Info   : ---------------------------------------------------------------
Info   : Reading input data ...
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.
================================================================================
```

2.1 Arguments

2.1.1 Input Data

`-n` *integer* [Input data]
Number of polyhedra of the tessellation, except for regular morphologies (cubes, 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}`). Regular morphologies can also be obtained: cubes (`cube`), dodecahedra (`dodeca`) and truncated octahedra (`tocta`), in which cases 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`.

For specifying a particular set of polyhedron centres, use '`-centrecoo`' instead of '`-id`' and '`-morpho`',

`-centrecoo` *file_name* [Input data]
Specify the coordinates of the polyhedron centres. Give as argument the name of the file containing the $3 * n$ coordinates.
Possible values: `any`. Default value: `none`.

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

`-load` *input_type file_name* [Input data]
Load a tessellation from a file. Provide the type of input data (must be '`tess`') and the file name.
Possible values: `"tess"` `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 Tessellation Options

`-dsize` *real real real* [Option]
Specify the domain size in the three directions of space.
Possible values: `any` > `0`. Default value: `1 1 1`.

`-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 (Appendix A [Mathematical expressions], page 35). 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 shift distance and an identifier for the randomization.
Possible values: `any > 0 any`. Default value: `none`.

2.1.4 Output options

`-format` *`char_string`* [Option]
Specify the format of the output file(s). To get several format, combine them with '`,`'.
Possible values: `tess, oin, geo`. Default value: `tess,oin`.

2.1.5 Post-Processing Options

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

`-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`'.

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

2.2 Output Files

2.2.1 Tessellation

- tessellation file: '`.tess`'

  It contains an exhaustive description of the tessellation.
- 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 25).
- 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`.)

2.2.2 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`

2.2.3 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

1. Generate a tessellation in 1000 polyhedra, with identifier = 1.

   ```
   $ neper -T -n 1000 -id 1
   ```
2. Like 1., but consider a domain $(3 * 0.33 * 1)$ in size.

   ```
   $ neper -T -n 1000 -id 1 -dsize 3 0.33 1
   ```
3. Like 1., but scale the tessellation once generated, and sort the grain according to their x coordinate.

   ```
   $ neper -T -n 1000 -id 1 -scale 3 0.33 1 -sort poly "cenx"
   ```
4. Generate a columnar tessellation along x in 1000 polyhedra, with identifier = 1.

   ```
   $ neper -T -n 1000 -id 1 -morpho columnarx
   ```
5. Generate a regular tessellation into truncated octahedra, of 5 * 5 * 5 grains (approximately).

   ```
   $ neper -T -reg tocta 5
   ```

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 conforms 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 (*`cl`*)*. 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, `rcl`, is also defined: $\texttt{rcl} = 2 * \texttt{cl}/(\texttt{average\_poly\_volume}^{1/3})$.

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[1], for parallel finite element simulations. 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`').

[1] Each partition being assigned to a processor in the finite element simulation, 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  (beforehand: neper -T -n 10 -id 1)

=======================    N   e   p   e   r    =======================
Info   : A 3D random polycrystal generator for the finite element method
Info   : Version 1.9.2 (18 Sept 2011)
Info   : (compiled with: gsl, libmatheval, libscotch)
Info   : Loading initialization file '/home/rquey/.neperrc'...
Info   : ---------------------------------------------------------------
Info   : MODULE -FM run with arguments:
Info   : [ini file] -nset faces -mo 2 -gmsh /home/rquey/bin/gmsh
         -partrenumber 1 -mesh3dalgo netg/gmsh,netg/gmne
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   :   - Testing tessellation ...
Info   :   - Deleting small edges ... (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% (0.26/0.26|0.85 - 12|87)
Info   :   - 3D meshing ... 100% (1/1|0.54/0.62|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:     1860
Info   :     > Elt  number:     1047
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: 17.922 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 (any 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 (*cl*/*pl*). Use this option if you want to choose a different length.
Possible values: `any`. Default value: `-sel` *cl*/*pl*.

`-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 by commas, e.g. *mesh1/opti1,mesh1/opti2,mesh2/opti2*. The 2D and 3D meshings are carried out using the Gmsh[1] and Netgen[2] 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.

[1] 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.

[2] J. Schoberl, 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, separated by commas.
Possible values: `made`, `mead`, `dela`, `fron`, and `combinations`. Default value: `default (= fron,made)`.

`-mesh3dalgo` *char_string* [Option]
Specify the 3D meshing algorithm. Multimeshing is allowed by providing several algorithms, separated by commas.
Possible values: `netg`, `netg/netg`, `netg/gmsh`, `netg/gmne`, and `combinations`. 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-mentionned 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 (*cl/pl*). Use this option if you want to choose a different length.
Possible values: `any`. Default value: `-sel` *cl/pl*.

`-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 >= 1`. Default value: `2`.

3.1.6 Mesh Partitioning Options

Mesh partitionning is achieved through the libScotch library[3]. 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`.

[3] 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 (point to volume elements), or any combination of them.
Possible values: `0, 1, 2, 3, and combinations`. 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 Zébulon, and `fev` for Fem-Evps. For the tessellation geometry, the available formats are: `tess` and `geo`. Give as argument the list of formats combined by commas.
Possible values: `anyone of the above list`. Default value: `msh`.

`-nset` *char_string* [Option]

Specify the node sets to provide (combine with commas), among: `faces`, `edges`, `vertices` for all domain faces, edges and vertices; `facebodies` and `edgebodies`, for all face and edge bodies; then for individual entities: `[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. Specify the nset names combined by commas.
Possible values: `any`. Default value: `faces`.

`-faset` *char_string* [Option]

Fem-Evps format only. Specify the surfaces to provide, in the '`.surf`' file, among: `faces` (for all), and `[x-z][0,1]` (combine with commas).
Possible values: `any`. Default value: `faces`.

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`.

`-mesh3dclconv` *real* [Secondary option]
Maximum tolerated difference between the characteristic length `cl` and the average element length (for each polyhedron). Neper tries its best to get the average element size to match `cl`. 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 third-party software formats:

- Gmsh format: file '`.msh`'
- Abaqus format: file '`.inp`'
- 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

- tessellation file: '`.tess`'

  It contains an exhaustive description of the tessellation.

- 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`.)

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`

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

1. *Mesh parameters.* Mesh tessellation '`n10-id1.tess`' with *rcl* = 0.8 and in 2nd-order elements.

   ```
   $ neper -FM n10-id1.tess -rcl 0.8 -order 2
   ```

2. *Regularization.* Like 1., but regularize the geometry before meshing, with *maxff* = 20, and save the regularized tessellation and mesh under files '`n10.*`'. Save the mesh in both Gmsh ('`.msh`') format and Abaqus ('`.abq`') format.

   ```
   $ neper -FM n10-id1.tess -maxff 20 -rcl 0.8 -order 2
     -format tess,msh,abq -o n10
   ```

3. *Multimeshing.* Like 2., but 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
   ```

4. *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
   ```

5. *Heterogeneous mesh refinement.* Mesh tessellation '`n100-id1.tess`' with heterogeneous mesh refinement: $rcl = 1.5$ for the surface grains, and $rcl = 0.2$ for the inner grains. Use geometry regularization.

```
$ neper -FM n100-id1.tess -maxff 20 -rcl 0.2
  -dbound "body<1" -dboundrcl 1.5
```

6. *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
```

7. *Remeshing.* Perform remeshing of mesh '`n10.msh`', whose corresponding tessellation file is '`n10.tess`', with $rcl = 0.5$. Save the results as files '`n10-b.*`'.

```
$ neper -FM -remesh n10.msh -remeshtess n10.tess -rcl 0.5
  -o n10-b
```

8. *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
```

9. *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 stairstepped shapes. The input file is a tessellation file ('`.tess`'), as provided by module -T, 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 -n 10 -id 1

========================    N   e   p   e   r    ======================
Info   : A 3D random polycrystal generator for the finite element method
Info   : Version 1.9.2 (18 Sept 2011)
Info   : (compiled with: gsl, libmatheval, libscotch)
Info   : Loading initialization file '/home/rquey/.neperrc'...
Info   : ---------------------------------------------------------------
Info   : MODULE -MM run with arguments:
Info   : [ini file] (none)
Info   : [com line] -n 10 -id 1
Info   : ---------------------------------------------------------------
Info   : Mapped meshing ...
Info   :   - Generating mesh ...
Info   :   - Searching elsets ...
Info   :   - Writing mapped mesh ...
Info   :     [o] Writing file 'n10-id1.msh' ...
Info   :     [o] Wrote file 'n10-id1.msh'.
Info   : Writing results ...
Info   :     [o] Writing file 'n10-id1.oin' ...
Info   :     [o] Wrote file 'n10-id1.oin'.
Info   : Elapsed time: 0.109 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 two following ones (the domain is a unit cube):

`-n` *integer* [Input data]
Number of polyhedra of the tessellation (for standard and periodic tessellations), or
Mean number of polyhedra per unit volume (for subdomain-type tessellations).
Possible values: `any`. Default value: `none`.

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

For specifying a particular set of polyhedron centres, use `-centrecoo` instead of `-id`,

`-centrecoo` *file_name* [Input data]
Specify the coordinates of the polyhedron centres. Give as argument the name of the file containing the $3 * n$ coordinates.
Possible values: `any`. Default value: `none`.

For regular tessellations, the required input data is,

`-regular` *char_string integer* [Input data]
Morphology and number of polyhedra along an edge of the domain. The morphology must be: tocta (truncated octahedra).
Possible values: `"tocta" any`. Default value: `none`.

4.1.2 General Options

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

4.1.3 Tessellation Options

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

`-ttype` *integer* [Option]
Specify the type of tessellation (applies to tessellations built with `(n, id)`, not by module -T ('`.tess`' file)). Set the option to: `0` for a standard tessellation, `1` for a periodic tessellation, `2` for a subdomain-type tessellation or `3` for a subdomain-type tessellation, but with a regular density of polyhedron centres.
Possible values: `0 to 3`. Default value: `0`.

4.1.4 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`.

4.1.5 Output Options

`-nset` *char_string* [Option]
Specify the node sets to provide (combine with commas), among: `faces`, `edges`, `vertices` for all domain faces, edges and vertices; `facebodies` and `edgebodies`, for all face and edge bodies; then for individual entities: `[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. Specify the nset names combined by commas.
Possible values: `any`. Default value: `faces`.

`-faset` *char_string* [Option]
Specify the domain surfaces to provide (use '`faces`' for all faces). [Zébulon format only]
Possible values: `faces, [x-z][0,1] and combinations`. Default value: `faces`.

4.2 Output Files

4.2.1 Mesh

The mesh can be written in the following third-party software formats:

- Gmsh format: '`.msh`'
- Abaqus format: file '`.inp`'
- 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 25).

4.3 Examples

- Mesh tessellation '`n0-id1.tess`' with *msize* = 25.
  ```
  $ neper -MM n10-id1.tess -msize 25
  $ neper -MM -n 10 -id 1 -msize 25 (faster)
  ```
- Like 1., and generate the node sets for the faces and edges of the domain.
  ```
  $ neper -MM -n 10 -id 1 -msize 25 -nset faces,edges
  ```
- Generate and mesh a periodic tessellation
  ```
  $ neper -MM -n 10 -id 1 -ttype 1
  ```

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 (Bonge, 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 n10-id1.oin

========================    N   e   p   e   r    ======================
Info   : A 3D random polycrystal generator for the finite element method
Info   : Version 1.9.2 (18 Sept 2011)
Info   : (compiled with: gsl, libmatheval, libscotch)
Info   : Loading initialization file '/home/rquey/.neperrc'...
Info   : ---------------------------------------------------------------
Info   : MODULE  -O run with arguments:
Info   : [ini file] -crysym cubic
Info   : [com line] n10-id1.oin
Info   : ---------------------------------------------------------------
Info   :     [i] Parsing file 'n10-id1.oin' ...
Info   :     [i] Parsed file 'n10-id1.oin'.
Info   :     [o] Writing file 'n10-id1.ori' ...
Info   :     [o] Wrote file 'n10-id1.ori'.
Info   : Elapsed time: 0.003 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

`-crysym` *`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-mentionned 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 Zébulon `geof` and the Fem-Evps `fev`.
Possible values: `anyone of the above list`. 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, '`-crysym`' 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

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

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

- *Orientation generation.* Generate a set of crystallographic orientations from (`n`, `id`), represented as Euler angles in Kocks convention.

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

- *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 -crysym cubic -col R
```

6 Mesh and Data Visualization: neper -VS

Module -VS is the Neper visualization module, with which tessellations and meshes can be rendered as publication-quality images. The entity colours are specified by the user, enabling post-processing. The input files are typically a tessellation file and / or a mesh file, and a file providing the colours to render the plotted data. The output file is a PNG file.

Contrary to the other modules, this module executes the provided argument successively. Typically, using module -VS first consists in loading a tessellation and / or a mesh (options starting by '`-load`'), as well as data to be plotted on them. The latter can be colours for tessellation polyhedra and mesh elements, and coordinates for the nodes (options starting by '`-data`'). Specific tessellation polyhedra and edges, or mesh elements can be set to be visible on the rendered image (options starting by '`-show`'). The way they are plotted can be set up (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 -loadmesh n10-id1.msh -loadtess n10-id1.tess \
              -dataelsetcolour n10-id1.col -showelt all -print img

========================    N   e   p   e   r    ======================
Info   : A 3D random polycrystal generator for the finite element method
Info   : Version 1.9.2 (18 Sept 2011)
Info   : (compiled with: gsl, libmatheval, libscotch)
Info   : Loading initialization file '/home/rquey/.neperrc'...
Info   : ---------------------------------------------------------------
Info   : MODULE -VS run with arguments:
Info   : [ini file]
Info   : [com line] -loadmesh n10-id1.msh -loadtess n10-id1.tess
         -dataelsetcolour n10-id1.col -showelt all -print img
Info   : ---------------------------------------------------------------
Info   : Loading mesh ...
Info   :     [i] Parsing file 'n10-id1.msh' ...
Info   :     [i] Parsed file 'n10-id1.msh'.
Info   : Reconstructing mesh ...
Info   : Loading tessellation ...
Info   :     [i] Parsing file 'n10-id1.tess' ...
Info   :     [i] Parsed file 'n10-id1.tess'.
Info   :     [i] Parsing file 'n10-id1.col' ...
Info   :     [i] Parsed file 'n10-id1.col'.
Info   : Printing mesh ...
Info   :     [o] Writing file 'img.pov' ...
Info   :   - Preparing mesh data ...
Info   :   - Reducing data ...
Info   :     > Number of elements   reduced by 64% (to 376).
Info   :     > Number of elt faces  reduced by 72% (to 428).
Info   :     > Number of face edges reduced by  0% (to 1284).
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   : Elapsed time: 1.969 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 and Mesh Data Loading

Here are options to load data on the tessellation:

`-datapolycolour` *file_name* [Option]
Load the tessellation polyhedron colours from a file. The file must contain the list of RGB levels (3 values between `0` and `255` for each polyhedron).
Possible values: `any`. Default value: `none`.

Here are options to load data on the mesh:

`-datanodecoo` *file_name* [Option]
Load specific node coordinates.
Possible values: `any`. Default value: `none`.

`-dataeltcolour` *file_name* [Option]
Load the element colours.
Possible values: `any`. Default value: `none`.

`-dataelsetcolour` *file_name* [Option]
Load the elset colours (same effect as '`-datapolycolour`').
Possible values: `any`. Default value: `none`.

6.1.3 Show Settings

`-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: *cenx*, *ceny*, *cenz*, *volume*, *true*, *body*, and *id*.
Possible values: `any`. Default value: `all if tess loaded (and no mesh) and nothing -show'd`.

`-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: *cenx*, *ceny*, *cenz*, *length*, *true*, *body*, *id*, *poly_true*, *poly_body*, and *poly_shown*.
Possible values: `any`. Default value: `none`.

`-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: *cenx*, *ceny*, *cenz*, *volume*, *elset_true*, *elset_body*, *elset_id*, and *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`.

`-showelt1d` *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*, and *elt3d_shown*.
Possible values: `any`. Default value: `none`.

`-showelt1din` *logical* [Secondary option]
This is an extension of option '`-showelt1d`' that enables to simulate 1D elements at the intersection between grains within a cut polycrystal.
Possible values: `0 or 1`. Default value: `0`.

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

6.1.4 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`.

6.1.5 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`.

`-printeltedgerad` *real* [Option]
Specify the radius of the element edges.
Possible values: `any`. Default value: `see_the_code`.

`-printelt1dedgerad` *real* [Option]
Specify the radius of the 1D element edges.
Possible values: `any`. Default value: `see_the_code`.

`-printedgerad` *real* [Option]
Specify the radius of the tessellation edges.
Possible values: `any`. Default value: `see_the_code`.

6.1.6 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`.

6.2 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 invoquing POV-Ray as follows (see the POV-Ray documentation for details and further commands):

```
$ povray +Ifile.pov +Wimage_width +Himage_height -D      .
```

6.3 Examples

1. Print tessellation '`n10-id1.tess`' with the colours given in file '`n10-id1.col`' to render the polyhedra.
```
$ neper -VS -loadtess n10-id1.tess -datapolycolour n10-id1.col
  -print image
```
2. Print mesh '`n10-id1.msh`' with the colours given in file '`n100-id1.col`' to render the elements.
```
$ neper -VS -loadmesh n10-id1.msh -dataeltcolour elements.col
  -print image
```
3. Print mesh '`n100-id1.msh`' with the colours given in file '`n100-id1.col`' to render the element sets. Plot only the body polyhedra (or element sets).
```
$ neper -VS -loadmesh n100-id1.msh -dataelsetcolour n100-id1.col
  -showelset "body>0" -print image
```
4. Print mesh '`n100-id1.msh`' with the colours given in file '`n100-id1.col`' to render the element sets. Plot only the body polyhedra (or element sets).
```
$ neper -VS -loadmesh n100-id1.msh -dataelsetcolour n100-id1.col
  -showelset "body>0" -print image
```
5. Like 4, and plot the 1D elements.
```
$ neper -VS -loadmesh n100-id1.msh -dataelsetcolour n100-id1.col
  -showelset "body>0" -showelt1d elt3d_shown -print image
```
6. Like 4, and set up the camera so that the mesh is seen along the y axis.
```
$ neper -VS -loadmesh n100-id1.msh -dataelsetcolour n100-id1.col
  -showelset "body>0" -showelt1d elt3d_shown -cameracoo meshcentre
  -cameracooy 15 -print image
```

7. Like 6, and produce an image of better quality: 2000 x 1500 pixels, with antialiasing.
```
$ neper -VS -loadmesh n100-id1.msh -dataelsetcolour n100-id1.col
  -showelset "body>0" -showelt1d elt3d_shown -cameracoo meshcentre
  -cameracooy 15 -imagesize 2000 1500 -imageantialias 2 -print image
```
8. Like 7, but plot the element edges a bit thicker, 0.001 in radius.
```
$ neper -VS -loadmesh n100-id1.msh -dataelsetcolour n100-id1.col
  -showelset "body>0" -showelt1d elt3d_shown -cameracoo meshcentre
  -cameracooy 15 -imagesize 2000 1500 -imageantialias 2
  -printelt1dedgerad 0.001 -print image
```
9. Like 8, and clip the mesh at different z coordinates: from 0 to 1 by step of 0.1. Generate an image for each value of z.
```
$ neper -VS -loadmesh n100-id1.msh -dataelsetcolour n100-id1.col
  -cameracoo meshcentre -cameracooy 15 -printelt1dedgerad 0.001
  -imagesize 2000 1500 -imageantialias 2 -loop Z 0 0.1 1
  -showelt "(elset_body>0)||(cenz<Z)"
  -showelt1d elt3d_shown -print image-Z -endloop
```

Appendix A Mathematical and Logical Expressions

A.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[1]:

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 multiplication (`'/'`) 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.

A.2 Logical expressions

The logical operators supported are: $=$ (`==`), $\neq$ (`!=`), $\geq$ (`>=`), $\leq$ (`<=`), $>$ (`>`), $<$ (`<`), AND (`&&`) and OR (`||`).

[1] Taken from the `libmatheval` documentation.

Appendix B Versions

```
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 >=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 -eulerangleconvention (Bunge, Roe & Kocks);
  new output formats mae and geof (option -format).
- manual: some corrections.

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

Appendix C GNU General Public License

GNU General Public License

Version 3, 29 June 2007

Preamble

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