Supplementary Online Material for article
Minkowski Tensors of Anisotropic Spatial Structure
to appear in The New Journal of Physics (2013)

User Manual for the Minkowski Tensor Package *Karambola*

Karambola is a simple C++ program to calculate all linearly independent Minkowski tensors up to rank two of a three-dimensional body from a triangulated representation of its bounding surface. It implements the algorithms derived in sections 2.1 to 2.8 and summarized in Table 2 of the above mentioned research article.

Overview

Karambola is a program to calculate the Minkowski Tensors of three-dimensional bodies, represented by triangulations of their bounding surfaces. The specific format for triangulations of the bounding surfaces is the simple ASCII .poly file format, detailed below, that simply provides a list of points and a list of triangles.

If the body is a finite compact set, its bounding surface is a closed surface; this is the standard case for which Minkowski tensors are defined. However, *karambola* also works with triangulations that do not represent closed surfaces, but rather have open boundaries. This case is relevant for the computation of the Minkowski tensors of a representative unit cell of a periodic structure, or for the experimentally relevant case where only a finite and assumed to be representative subset of a larger structure (a window of observation) is available.

Karambola also allows for the computation of subsets of a given structure; for this purpose the surface triangulation is subdivided by assigning an integer number called *label*. to each triangle. All triangles with the same value of *label* are seen as defining the subset whose Minkowski tensors are computed. This functionality is particularly useful for the local analysis through a so-called *Minkowski map*.

Brief description of the implementation

Karambola reads in a .poly file and stores this data in a `Triangulation` class.

The Calc_Options class stores the configuration data such as whether to calculated labelled Minkowski Tensors (MT), which tensors to calculate, etc.

In order to calculate the MT, Karambola generates look-up tables that allow the efficient lookup of the associations vertex→polygon and polygon→polygon.

Before computing Minkowski tensors, Karambola performs that basic consistency and validation checks on the triangulation. In particular, *karambola* tests for correctness of the triangle neighbourhoods (what is required depends on the tensors to be computed). It also computes and records records smallest and largest edge lengths and triangle areas.

After that, the scalar, vector and matrix Minkowski Functionals are calculated based on the definitions and algorithms of sections 2.1 to 2.8 and Table 2 of the article mentioned above.

Then the results are printed either in the terminal or in files.

As many analyses will require the eigenvalues or eigenvectors of the Minkowski tensors, the eigensystems of the rank-two Minkowski Tensors are calculated and printed to files.

Installation

The karambola package is installed by extracting the tar-ball into a subdirectory and using the command `make` to compile the program. The program is coded to ISO-C++ standards and should be easily portable to most platforms. On linux systems, use

```
bunzip2 karambola-NJP.tar.bz2
tar xvf karambola-NJP.tar
cd karambola-NJP
make
```

The program requires the GSL library http://www.gnu.org/software/gsl/ (for example, the libgsl-dev or libgsl-devel package on Linux).

Usage

Karambola is a command-line driven program. Use the following syntax:

```
./karambola input-file.poly {--labels | --nolabels} [options]
```

The label flag is a compulsary argument to the program.

`--nolabels`	ignore the labels in the input file, if existent
`--labels`	read label attributes from input-file and compute label-wise tensors

The program aborts with an error message if the file has no labels and the `--labels` option is set.

By default, *Karambola* calculates the full set of Minkowski Tensors provided in Table 2 of the journal reference. If you like to compute a single tensor only, you can use the `--compute w???` option, for example, `--compute w102`.

Not all Minkowski Tensors can be calculated for any given input file, e.g. depending on wether the triangulation represents a closed bounding surface. If calculating the Minkowski Tensors for a file is not possible because of incomplete neighborhoods, Karambola will indicate that. If, however, you want to calculate the MT by stubbornly applying the formulae nevertheless, you can use the `--force w???` options:

```
--force w000          --force w200
--force w300          --force w010
--force w210          --force w310
--force w010          --force w210
--force w310          --force w202
```

For all but the translation-invariant Minkowski tensors, the resulting values depend on the choice of origin. By default, the origin is the point (0,0,0) in the same coordinate system as the coordinates of the points of the triangulation. The option `--reference_centroid`, the tensors are calculated in reference frame where the origin is set to the corresponding curvature centroid $W_\nu^{1,0}(K)/W_\nu(K)$ of the body K, see section 2.4 of the NJP article. If the keyword -labels is used in conjunction with `--reference_centroid`, then the origin is set individually for each subset of the data with the same `label` attribute.

The name of the output folder is controlled by the option

```
--output outputfoldername            or
-o outputfoldername
```

If this option is not set, Karambola creates a folder named `inputfilename_mink_val` into which the outputfiles will be written.

Description of the input file format .poly

A .poly file is a simple ASCII file that consists of two sections, separated by the keywords "POINTS", "POLYS", and "END".

The second section defines the actual polygons. Each polygon is introduced by a number, and a colon (:), followed by references to the vertices (integers ≥ 1). While karambola reads the poly file, each polygon is triangulated in a simple way. The first vertex is connected to every other vertex of the polygon, so that you get n-2 triangles, where n is the number of vertices of a triangle. Vertices are given in such order that the normal for each triangle of the polygon is defined by

$$\text{normal} = \frac{(\text{vertex}_{i+1} - \text{vertex}_1) \times (\text{vertex}_{i+2} - \text{vertex}_1)}{|(\text{vertex}_{i+1} - \text{vertex}_1) \times (\text{vertex}_{i+2} - \text{vertex}_1)|} \quad , \quad i = 1, ..., n-2 \qquad (1)$$

points to the outside of the object. '$\times$' indicated the cross product, and $|.|$ indicates the Euclidean norm. If the normal points to the inside, the volume and the mean curvature are negative.

To indicate a closed polygon, the character "<" is added. Non-closed polygons are presently unsupported; karambola ignores the request to construct an open polygon and constructs a closed one.

If you want to label your polygons you can do this with the color option: After the character "<" you can add a "c" which stands for color. Now you can add in parentheses four numbers separated by a comma. The first three are not used by karambola. Usually you define with them a color for the polygons. The last number has to be an integer and and is used for the label. For each label, the Minkowski Functionals, Vectors and Tensors are calculated individually if you use the `--labels` option. (an error occurs if the file has no labels and the `--labels` option is set).

The actual coordinates of each vertex are defined in the first section; again, each vertex is introduced by positive and consecutive integers starting from 1 and a colon; coordinates are given as floating-point numbers.

Minimal example of a file describing a triangle labelled with '7' and a quadrangle labelled with '2':

```
POINTS
1: 0.000000000e+00 0.000000000e+00 0.000000000e+00
2: 1.000000000e+00 0.000000000e+00 1.000000000e+00
3: 0.000000000e+00 1.000000000e+00 1.000000000e+00
4: 1.000000000e+00 1.000000000e+00 2.000000000e+00
POLYS
1: 1 2 3 < c(0, 0, 0, 7)
2: 1 2 4 3 < c(0, 0, 0, 2)
END
```

Description of output file formats

Karambola creates a folder named inputfilename_mink_val or if the "--output" option is set a user defined folder, into which the outputfiles will be written. 15 outputfiles will be written:

- **surface_props:**
  in this file are some statistics: the shortest edge, longest edge, smallest area and largest area and for every label whether the surface is closed, shared with other labels or open.
  ATTENTION: if the triangulation contains very short edges or small faces in your data, numerical errors may affect the accuracy of the results significantly. In its current version, *karambola* calculates the minimal edge lengths and triangle areas, but does not abort if very short edges or very small triangles exist.
- **w000_w100_w200_w300:**
  into this file the results for the Minkowski Functionals are written.
- **w010_w110_w210_w310:**
  into this file the results for the Minkowski Vectors are written.
- **w020, w120, w220, w320, w102, 202:**
  into this files the results for the Minkowski Tensors are written.
- **w020_eigsys, w120_eigsys, w220_eigsys, w320_eigsys, w102_eigsys, 202_eigsys:**
  into this files the results for the Minkowski Tensor eigenvalues and eigenvectors are written.

Contributors and future updates

Karambola was developed at the Institute of Theoretical Physics at the Friedrich-Alexander University Erlangen-Nuremberg by the authors of the research article 'Minkowski tensors of anisotropic spatial structure' (NJP, 2013). The current version described in this manual was implemented by Fabian Schaller and Sebastian Kapfer.

Future updates and examples for applications will be made publicly available on the website www.theorie1.physik.uni-erlangen.de/karambola, which also provides current contact details for the developers.