

# Package ‘molaR’

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**Title** Dental Surface Complexity Measurement Tools

**Version** 0.3

**Description** Surface topography calculations of Dirichlet’s normal energy, relief index, and orientation patch count for teeth using scans of enamel caps. Importantly, for the relief index and orientation patch count calculations to work, the scanned tooth files must be oriented with the occlusal plane parallel to the x and y axes, and perpendicular to the z axis. The files should also be simplified, and smoothed in some other software prior to uploading into R.

**Depends** R (>= 2.10), alphahull, psych, geomorph, rgl

**License** ACM

**LazyData** true

**Suggests** knitr, rmarkdown, rglwidget

**VignetteBuilder** knitr

**NeedsCompilation** no

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|                   |                              |
|-------------------|------------------------------|
| clustered_patches | <i>A clustering function</i> |
|-------------------|------------------------------|

---

### Description

This function gathers linked faces into patches

### Usage

```
clustered_patches(Directional_Bin_Face_Pairs)
```

### Arguments

Directional\_Bin\_Face\_Pairs  
the bins of face directions clustered\_patches()

---

|                         |  |
|-------------------------|--|
| compute_energy_per_face | <i>Function will compute the DNE per face.</i> |
|-------------------------|--|

---

### Description

This will generate each Dirichlet's normal energy for each triangular face on the surface.

### Usage

```
compute_energy_per_face(plyFile)
```

### Arguments

plyFile            a stanford PLY file compute\_energy\_per\_face()

---

|                  |  |
|------------------|--|
| Directional_Bins | <i>This bins the faces into directional categories</i> |
|------------------|--|

---

### Description

bins into 8 directional categories on the basis of their orientations

### Usage

```
Directional_Bins(plyFile, rotation = 0)
```

### Arguments

|          |   |
|----------|---|
| plyFile  | a stanford PLY file                                     |
| rotation | the amount to rotate the specimen by Directional_Bins() |

---

|     |   |
|-----|---|
| DNE | <i>Calculate Dirichlet normal energy of a surface</i> |
|-----|---|

---

### Description

A function that calculates Dirichlet normal energy following the method of Bunn et al. (2011) Comparing Dirichlet normal surface energy of tooth crowns, a new technique of molar shape quantification for dietary inference, with previous methods in isolation and in combination. Am J Phys Anthropol 145:247-261 doi: 10.1002 ajpa.21489

### Usage

```
DNE(plyFile, outliers = 0.1)
```

### Arguments

|          |  |
|----------|--|
| plyFile  | An object of class 'mesh3d' and 'shape3d' with calculated normals                            |
| outliers | The percentile of Dirichlet energy density values to be excluded defaults to top 0.1 percent |

### Details

The function requires an object created by reading in a ply file utilizing either the read.ply or the read.AVIZO.ply function, with calculated normals.

Dirichlet normal energy is calculated on meshes that represent specimen surfaces and have already been simplified to 10,000 faces and pre-smoothed in a 3D data editing program.

The function does not include boundary vertices in the calculation, and therefore the analyzed surface cannot be closed (i.e., it must contain a hole). The function defaults to remove the top 0.1 percent of calculated energy densities as outliers. Mesh orientation does not affect for this calculation.

DNE3d

*Plot results of a DNE analysis of a surface***Description**

plotting function

**Usage**

```
DNE3d(DNE_File, setRange = c(0, 0), edgeMask = TRUE, outlierMask = TRUE,
      logColors = TRUE, showEdgePts = FALSE, fieldofview = 0, legend = TRUE)
```

**Arguments**

|             |  |
|-------------|--|
| DNE_File    | An object that stores the output of the DNE function   |
| setRange    | User-defined range for plotting color scheme, see Details  |
| edgeMask    | Logical that colors edge faces black to indicate their lack of contribution to the total Dirichlet normal energy             |
| outlierMask | Logical that colors outlier faces dark gray to indicate their lack of contribution to the Dirichlet normal energy            |
| logColors   | Logical that log transforms the color scheme   |
| showEdgePts | Logical that highlights the edge vertices in red to indicate their lack of contribution of the total Dirichlet normal energy |
| fieldofview | Passes an argument to par3d changing the field of view in degrees of the resulting rgl                                       |
| legend      | Logical indicating whether or not a legend should be displayed   |

**Details**

This function creates a heat map on the mesh surface corresponding to the Dirichlet normal energy of each face calculated by the DNE function. Hottest colors represent highest normal energy values

Dirichlet normal energies for the faces of a mesh surface tend to be positively skewed, with a small proportion of the faces contributing much of the total energy for the surface. When logColors is enabled the function colorizes based on the log transformed Dirichlet normal energies, allowing for finer resolution between faces near the mode of the energy per face distribution. Disabling logColors will display the untransformed Dirichlet normal energies.

The legend will update to reflect the other arguments chosen by the user. Colors currently display in the legend in bins, however the colors used in the displayed mesh surface are on a continuum. Ideally, the legend should reflect a continuous stretch of color from the lowest calculated Dirichlet normal energy to the highest. Future versions will adjust the legend to this more intuitive display.

By default, the function sets the lowest Dirichlet normal energy calculated among all faces to a cool color and the highest normal energy calculated among all faces to red, and then colors the remaining faces on a continuous color spectrum between these two end points using either absolute or log transformed Dirichlet normal energy values (depending on the status of logColors). Since the scale is relative to the energies of the input surface, visual comparisons cannot directly be made between multiple plots of different surfaces. The setRange argument allows users to define the minimum and maximum of the plotting color scheme and use it in multiple plots. This enables the direct comparison of different surfaces to one another with red equal to the user-defined maximum

and a cool color equal to the user-defined minimum. The user should choose reasonable bounds for the maximum and minimum that are near the maximum and minimum Dirichlet normal energies calculated for their surfaces. `setRange` will not accept negative values.

`fieldofview` is set to a default of 0, which is an isometric projection. Increasing it alters the degree of parallax in the perspective view, up to a maximum of 179 degrees.

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DNE\_Legend

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*Make legend for DNE3d plot*


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## Description

plotting subfunction

## Usage

```
DNE_Legend(start, end, colors, DNELabels, scaled = F, edgeMask = F,
           outlierMask = F, logColors = F)
```

## Arguments

|                          |  |
|--------------------------|--|
| <code>start</code>       | value for the legend to start with, i.e. bottom value  |
| <code>end</code>         | value for the legend to end with, i.e. top value   |
| <code>colors</code>      | range of values, defaulting to heat colors   |
| <code>DNELabels</code>   | values for the labels  |
| <code>scaled</code>      | logical indicating whether the values are scaled   |
| <code>edgeMask</code>    | logical indicating whether or not edges are being masked and that information to be included in the legend |
| <code>outlierMask</code> | logical indicating whether outliers are masked   |
| <code>logColors</code>   | logical indicating colors are on log scale   |

## Details

This is an internal function which builds a better DNE plot legend

The legend will reflect the elements used in the plot. This is an internal function. Users will have little need or call to interact with it.

---

|               |   |
|---------------|---|
| edge_vertices | <i>Function for finding the edge vertices</i> |
|---------------|---|

---

### Description

Function will sort through all the vertices of the surface and find the ones which are on the edge. This will be needed for identifying which should be masked and not included in the calculation of the final DNE value.

### Usage

```
edge_vertices(plyFile)
```

### Arguments

|         |                     |
|---------|---------------------|
| plyFile | a stanford PLY file |
|---------|---------------------|

```
edge_vertices()
```

---

|                      |  |
|----------------------|--|
| Equal_Vertex_Normals | <i>Important function for re-doing the vertex normals for the DNE calculation.</i> |
|----------------------|--|

---

### Description

The geomorph import function does not generate the correct vertex normals.

### Usage

```
Equal_Vertex_Normals(plyFile)
```

### Arguments

|         |                     |
|---------|---------------------|
| plyFile | a stanford PLY file |
|---------|---------------------|

```
Equal_Vertex_Normals()
```

---

|           |                          |
|-----------|--------------------------|
| ex_tooth1 | <i>4149_DU-LP-09_LM1</i> |
|-----------|--------------------------|

---

### Description

Lower M1 of a male mantled howler monkey, *Aloutta palliata*. Catalogue Number DU-LP 09

### Usage

```
ex_tooth1
```

**Format**

A list of five objects, as follows:  
vb, a 4 x 5118 dataframe.  
it, a 3 x 10000 dataframe.  
primitivetype, a character string  
material, a NULL field  
normals, a 4 x 5118 dataframe

**Source**

MorphoSource

**References**

[http://www.morphosource.com/index.php/Detail/SpecimenDetail/Show/specimen\\_id/22](http://www.morphosource.com/index.php/Detail/SpecimenDetail/Show/specimen_id/22)

---

|           |                   |
|-----------|-------------------|
| ex_tooth2 | 4147_DU-LP-07_LM1 |
|-----------|-------------------|

---

**Description**

Lower M1 of a female mantled howler monkey, *Aloutta palliata*. Catalogue Number DU-LP 07

**Usage**

ex\_tooth1

**Format**

A list of five objects, as follows:  
vb, a 4 x 5135 dataframe.  
it, a 3 x 9997 dataframe.  
primitivetype, a character string  
material, a NULL field  
normals, a 4 x 5135 dataframe

**Source**

MorphoSource

**References**

[http://www.morphosource.com/index.php/Detail/SpecimenDetail/Show/specimen\\_id/29](http://www.morphosource.com/index.php/Detail/SpecimenDetail/Show/specimen_id/29)

---

|            |  |
|------------|--|
| face_areas | <i>Function to calculate face areas.</i> |
|------------|--|

---

**Description**

This function calculates the area of each face on a ply file

**Usage**

```
face_areas(plyFile)
```

**Arguments**

|         |                                  |
|---------|----------------------------------|
| plyFile | a stanford PLY file face_areas() |
|---------|----------------------------------|

---

|              |                                      |
|--------------|--------------------------------------|
| Face_Normals | <i>Function to find Face Normals</i> |
|--------------|--------------------------------------|

---

**Description**

This function re-computes the face normals in a way consistent with MorphoTester.

**Usage**

```
Face_Normals(plyFile)
```

**Arguments**

|         |                                    |
|---------|------------------------------------|
| plyFile | a stanford PLY file Face_Normals() |
|---------|------------------------------------|

---

|                             |  |
|-----------------------------|--|
| index_paired_directed_faces | <i>Index of paired faces with directions</i> |
|-----------------------------|--|

---

**Description**

This does some heavy lifting to pull together faces which are paired together. This is needed for many later functions for compiling OPC

**Usage**

```
index_paired_directed_faces(plyFile)
```

**Arguments**

|         |  |
|---------|--|
| plyFile | a stanford PLY file<br>index_paired_directed_faces() |
|---------|--|



OPC

*Calculate orientation patch count of a surface***Description**

A function that bins patches of a mesh surface that share general orientation and sums the number of unique patches given certain parameters Modified into 3D from the original 2.5D method described by Evans et al. (2007) High-level similarity of dentitions in carnivorans and rodents. Nature 445:78-81 doi: 10.1038 nature05433

**Usage**

```
OPC(plyFile, rotation = 0, minimum_faces = 3, minimum_area = 0)
```

**Arguments**

|               |  |
|---------------|--|
| plyFile       | An object of classes "mesh3d" and "shape3d" with calculated normals                                      |
| rotation      | Rotates the file in degrees about the center vertical axis   |
| minimum_faces | Minimum number of ply faces required for a patch to be counted towards the total patch count             |
| minimum_area  | Minimal percentage of total surface area a patch must occupy to be counted towards the total patch count |

**Details**

The function requires an object created by reading in a ply file utilizing either the read.ply or the read.AVIZO.ply function

Orientation patch count is calculated on meshes that represent specimen surfaces and have already been downsampled to 10,000 faces and pre-smoothed in a 3D data editing program. Alignment of the point cloud will have a large effect on patch orientation and must be done in a 3D data editing program such as Avizo, or using the R package auto3dgm prior to creating and reading in the ply file. The occlusal surface of the specimen must be made parallel to the X- and Y-axes and perpendicular to the Z-axis.

The default for minimum\_faces is to ignore patches consisting of only a single face on the mesh. Changing the minimum\_area value will disable minimum\_faces.

OPC3d

*Plot results of OPC analysis of a surface***Description**

A function that produces a three-dimensional rendering of face orientation on a surface. The OPC function will identify the orientations of mesh faces and assign them to patches. It must be performed prior to using the OPC3d function.

## Usage

```
OPC3d(OPC_Output_Object, fieldofview = 0, legend = TRUE, binColors = hsv(h
    = (seq(10, 290, 40)/360), s = 0.9, v = 0.85), patchOutline = FALSE,
    outlineColor = "black", maskDiscard = FALSE, minimum_faces = 3)
```

## Arguments

|                   |   |
|-------------------|---|
| OPC_Output_Object | An object that stores the output of the OPC function  |
| fieldofview       | Passes an argument to par3d changing the field of view in degrees of the resulting rgl window |
| legend            | Logical indicating whether or not a legend should be displayed                                |
| binColors         | Allows the user to change the colors filled in for each directional bin                       |
| patchOutline      | logical whether or not to outline the patches   |
| outlineColor      | parameter designating which color to outline the patches in                                   |
| maskDiscard       | logical indicating whether to discard the unused patches                                      |
| minimum_faces     | value for the minimum number of faces a patch must contain to avoid being discarded           |

## Details

This function will assign a uniform color to all faces on the mesh surface that share one of the 8 orientations identified by the OPC function. The function returns a colored shade3d of the mesh so that patches can be visually inspected. Future versions will include the option to black out patches not included in the orientation patch count.

fieldofview is set to a default of 0, which is an isometric projection. Increasing it alters the degree of parallax in the perspective view, up to a maximum of 179 degrees. colors will support any vector of 8 colors, in any coloration scheme. Default draws from the hsv color space to evenly space color information, however user can supply a list of RGB values, character strings, or integers in place.

---

OPCr

*Calculate average orientation patch count after several rotations*

---

## Description

A function that calls OPC iteratively after rotating mesh a selected number of degrees around the Z-axis following Evans and Jernvall (2009) Patterns and constraints in carnivoran and rodent dental complexity and tooth size. J Vert Paleo 29:24A

## Usage

```
OPCr(plyFile, Steps = 8, stepSize = 5.625, minimum_faces = 3,
    minimum_area = 0)
```

**Arguments**

|               |  |
|---------------|--|
| plyFile       | An object of classes 'mesh3d' and 'shape3d' with calculated normals                                    |
| Steps         | Number of iterations to run the OPC function on the mesh   |
| stepSize      | Amount of rotation in degrees about the Z-axis to adjust mesh surface by between each iteration of OPC |
| minimum_faces | Argument to pass to the OPC function   |
| minimum_area  | Argument to pass to the OPC function   |

**Details**

The function requires an object created by reading in a ply file utilizing either the read.ply or the read.AVIZO.ply function, with calculated normals.

Default number of Steps is 8, with a stepSize of 5.625 degrees, following the original definition of OPCR.

See the details for the OPC function for more information about preparing mesh surfaces and the effects of minimum\_faces and minimum\_area.

---

patches\_for\_each\_direction

*Function for gathering the patches for each direction*

---

**Description**

This function will gather the patches in each of the 8 bins and ready it for patches\_for\_each\_direction()

**Usage**

```
patches_for_each_direction(indexed_pairs)
```

**Arguments**

|               |                         |
|---------------|-------------------------|
| indexed_pairs | Pairs of touching faces |
|---------------|-------------------------|

---

patches\_per

*A function for patches within each face*

---

**Description**

this gets some important information out of each patch

**Usage**

```
patches_per(patch_details, plyFile, minimum_faces = 3, minimum_area = 0)
```

**Arguments**

|               |  |
|---------------|--|
| patch_details | information on each patch                            |
| plyFile       | a stanford PLY file                                  |
| minimum_faces | minimum number of faces in each counted patch        |
| minimum_area  | minimum area for a patch to be counted patches_per() |

---

|               |  |
|---------------|--|
| patch_details | <i>Function for gathering patch details for each Orientation patch</i> |
|---------------|--|

---

### Description

This function does some simple math to let us know about the patches

### Usage

```
patch_details(clusterlist, plyFile)
```

### Arguments

|             |  |
|-------------|--|
| clusterlist | a list of faces in the cluster patch_details() |
| plyFile     | a stanford PLY file                            |

---

|                |   |
|----------------|---|
| read.AVIZO.ply | <i>Read mesh data from ply files saved by AVIZO</i> |
|----------------|---|

---

### Description

A function that reads Stanford ply files as saved by the 3D data visualization software Avizo

### Usage

```
read.AVIZO.ply(file, ShowSpecimen = TRUE, addNormals = TRUE)
```

### Arguments

|              |  |
|--------------|--|
| file         | An ASCII PLY file generated by Avizo   |
| ShowSpecimen | Logical indicating whether or not the mesh should be displayed   |
| addNormals   | Logical indicating whether or not normals of mesh vertices should be calculated and appended to object |

### Details

If ShowSpecimen is True, a gray shade3d of the mesh is generated in a new rgl window for previewing the specimen. When saving to the ply file type, Avizo inserts additional property parameters into the file heading that sometimes describe various components of the mesh. These additional properties cause the read.ply function native to the geomorph package to fail. This function properly reads ply files generated by Avizo (like read.ply) and can be stored as an object accepted as input in the other molaR functions. Ply files generated through other software (such as MeshLab) can be read using read.ply.

---

remove\_boundary\_faces    *Remove boundary faces*

---

### Description

Important function for masking the edge faces

### Usage

```
remove_boundary_faces(Energy_Per_Face_Values, plyFile)
```

### Arguments

|                        |   |
|------------------------|---|
| Energy_Per_Face_Values | information on E per face remove_boundary_faces() |
| plyFile                | a stanford PLY file                               |

---

remove\_outliers    *Mask outliers on some faces*

---

### Description

This function will block out the top 0.1 percent of the faces

### Usage

```
remove_outliers(Energy_values, X)
```

### Arguments

|               |   |
|---------------|---|
| Energy_values | energy density values on faces                        |
| X             | percentile above which to remove<br>remove_outliers() |

---

RFI    *Calculate Boyer's (2008) relief index for a surface*

---

### Description

A function that calculates relief index following Boyer (2008) Relief index of second mandibular molars is a correlate of diet among prosimian primates and other mammals. J Hum Evol 55:1118-1137 doi: 10.1016/j.jhevol.2008.08.002

### Usage

```
RFI(plyFile)
```

**Arguments**

plyFile                    An object of classes 'mesh3d' and 'shape3d'

**Details**

The function requires an object created by reading in a ply file utilizing either the read.ply or the read.AVIZO.ply function, with calculated normals.

Relief index is calculated by the ratio of three-dimensional surface area to two dimensional area on meshes that represent specimen surfaces and have already been pre-smoothed in a 3D data editing program. Alignment of the point cloud will have a large effect on patch orientation and must be done in a 3D data editing program or auto3dgm prior to creating and reading in the ply file. The mesh must be oriented such that the occlusal plane is parallel to the X- and Y-axes and perpendicular to the Z-axis.

---

RFI3d

---

*Plot 3D and 2D areas of a mesh used to calculate relief index*


---

**Description**

A function that plots a three-dimensional model of the mesh surface and includes a footprint of the two-dimensional area for visual comparison.

**Usage**

```
RFI3d(RFI_Output, displace = "Up", SurfaceColor = "gray",
      FootColor = "red", fieldofview = 0, Transparency = 1, legend = F)
```

**Arguments**

|              |  |
|--------------|--|
| RFI_Output   | An object that stores the output of the RFI function   |
| displace     | Moves the surface footprint up, down, or not at all  |
| SurfaceColor | changes the color of the 3D surface mesh   |
| FootColor    | changes color of the 2D surface footprint  |
| fieldofview  | Passes an argument to par3d changing the field of view in degrees of the resulting rgl window                        |
| Transparency | adjusts the transparency of the 3D mesh surface  |
| legend       | Logical indicating whether or not to include a legend of the colors chosen to represent the 3D surface and footprint |

**Details**

This function can help to visualize the three-dimensional and two dimensional areas that are used in calculating the relief index of a surface by displaying both at the same time. The RFI function must be performed first.

Transparency can be adjusted in a range from fully opaque (1) to fully transparent (0) in order to help visualize the footprint. The vertical placement of the footprint along the Z axis can be altered with displace depending on how the user wishes to view the surface, or on the original mesh orientation.

fieldofview is set to a default of 0, which is an isometric projection. Increasing it alters the degree of parallax in the perspective view, up to a maximum of 179 degrees.

---

vertex\_to\_face\_list     *function for making a list of faces on each vertex*

---

**Description**

crucial function for getting a list of faces which will gather the faces per vertex.

**Usage**

```
vertex_to_face_list(plyFile)
```

**Arguments**

plyFile             a stanford PLY file vertex\_to\_face\_list()

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