Package 'xvm'

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Title Read, Parse and Visualize 'XVG'/'XPM' Files from Molecular Dynamics

Version 0.0.1

Description

Provides tools for reading, parsing and visualizing simulation data stored in 'xvg'/'xpm' file formats (commonly generated by 'GROMACS' molecular dynamics software). Streamlines post-processing
and analysis of molecular dynamics ('MD') simulation outputs, enabling efficient exploration of molecular stability and conformational changes. Supports import of trajectory metrics ('RMSD', energy, temperature) and creation of publication-ready visualizations through integration with 'ggplot2'.

URL https://github.com/RightSZ/xvm, https://rightsz.github.io/xvm/

BugReports https://github.com/RightSZ/xvm/issues

Encoding UTF-8

RoxygenNote 7.3.2

Imports ggplot2, tidyr, ggnewscale, plotly

Suggests knitr, rmarkdown, ggpubr, stringr

VignetteBuilder knitr

License GPL (>= 3)

NeedsCompilation no

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Repository CRAN

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Contents

`plot_xpm` *plot xpm data*

Description

plot xpm data using ggplot2

Usage

```
plot_xpm(xpm_data, interpolate = FALSE)
```

Arguments

`xpm_data`	a xpm object returned by read_xpm
`interpolate`	logical indicating whether to use raster interpolation (TRUE) or discrete tiles (FALSE). Default is FALSE.

Value

a ggplot2 object

Examples

```
library(xvm)
xpm_file_path <- system.file("extdata/gibbs.xpm", package = "xvm")
xpm_data <- read_xpm(xpm_file_path)
plot_xpm(xpm_data) # plot the xpm data using plot_xpm() function
```

`plot_xpm_3d` *generate 3d scatter plot from xpm Data*

Description

creates 3d visualization of xpm data with scatter plot.

Usage

```
plot_xpm_3d(xpm_data, reversescale = FALSE, point_size = 2)
```

Arguments

xpm_data	a xpm object (from read_xpm()) or list containing parsed objects.
reversescale	whether to reverse the color scale; default is FALSE
point_size	the size of the points in the scatter plot; default is 2

Value

a plotly object

Examples

```
library(xvm)
xpm_file_path <- system.file("extdata/gibbs.xpm", package = "xvm")
xpm_data <- read_xpm(xpm_file_path)
plot_xpm_3d(xpm_data) # plot 3D scatter plot from xpm file
```

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plot_xpm_facet *generate faceted plots from xpm Data*

Description

creates dual-panel visualizations of xpm data with scatter or area plots.

Usage

```
plot_xpm_facet(xpm_data, plot_type = "scatter")
```

Arguments

xpm_data	a xpm object (from read_xpm()) or list containing parsed objects.
plot_type	visualization type: "scatter" (default) or "area".

Value

a ggplot2 object with:

- Dual facets showing x/y axis relationships
- Automatic data transformation for visualization
- NULL if invalid plot_type specified

Examples

```
library(xvm)
xpm_file_path <- system.file("extdata/gibbs.xpm", package = "xvm")
xpm_data <- read_xpm(xpm_file_path)
plot_xpm_facet(xpm_data) # plot pseudo-3D from xpm file
```

plot_xvg *plot xvg data*

Description

plot xvg data using ggplot2

Usage

```
plot_xvg(xvg_data, title = NULL, subtitle = NULL, ...)
```

Arguments

xvg_data	xvg data object returned by read_xvg
title	chart title (default uses xvg file's title)
subtitle	chart subtitle (default uses xvg file's subtitle)
...	additional parameters passed to ggplot2::geom_line

Value

a ggplot2 object

Examples

```
library(xvm)
rmsd_file_path <- system.file("extdata/rmsd.xvg", package = "xvm")
rmsd_data <- read_xvg(rmsd_file_path)
plot_xvg(rmsd_data) # plot the xvg data using plot_xvg() function
```

read_xpm *read xpm files*

Description

This function reads xpm (X PixMap) files, validates their existence, and returns parsed data structures in a list format.

Usage

```
read_xpm(xpm_files)
```

Arguments

xpm_files	a character vector containing paths to one or more xpm files.

Details

The function performs the following operations:

1. Validates input type (must be character vector)
2. Checks for file existence and filters missing files with warnings
3. Reads valid files and parses them using `parse_xpm()`
4. Returns aggregated results in a named list

Value

list with the following components:

- data - Data frame containing matrix values with coordinates
- title - Chart title extracted from xpm
- legend - Legend text extracted from xpm
- x_label - X-axis label extracted from xpm
- y_label - Y-axis label extracted from xpm
- color_map - Named list mapping color codes to hex values
- color_values - Named list mapping color codes to numeric values

Examples

```
library(xvm)
# Retrieve the path to the example file included in the package
xpm_file_path <- system.file("extdata/gibbs.xpm", package = "xvm")
xpm_data <- read_xpm(xpm_file_path) # read the xpm file using read_xpm() function
names(xpm_data)
```

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read_xvg *read xvg files*

Description

read one or more GROMACS-generated xvg files

Usage

```
read_xvg(xvg_files, skip_comments = TRUE)
```

Arguments

xvg_files	character vector of xvg file paths
skip_comments	logical indicating whether to skip comment lines (default: TRUE)

Value

Named list containing xvg data, using filenames (without extension) as keys

Examples

```
library(xvm)
# Retrieve the path to the example file included in the package:
rmsd_file_path <- system.file("extdata/rmsd.xvg", package = "xvm")
rmsd_data <- read_xvg(rmsd_file_path) # read the xvg file using read_xvg() function
names(rmsd_data)
```

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