Package ‘xvm’

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

Version 0.0.2

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

Depends R (>= 4.1.0)

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

export_xvg *export xvg data object*

Description

write the data component of an xvg_data object (or multiple objects) to a delimited text file, controlled via the sep parameter rather than file extension detection.

Usage

```
export_xvg(xvg_data, file, sep = "\t", row.names = FALSE, merge = FALSE, ...)
```

Arguments

xvg_data An object of class xvg_data, or a list of xvg_data objects, as returned by read_xvg().

file Path to the output file (any extension is acceptable).

sep Field separator (e.g., "\t" for TSV, "," for CSV). Default is "\t".

row.names Logical, whether to write row names. Default is FALSE.

merge Logical, whether to merge multiple xvg_data objects before exporting. Default is FALSE.

... Additional arguments passed to write.table().

Value

Invisibly returns the path to the written file.

Examples

```
## Not run:
xvg <- read_xvg(system.file("extdata/rmsd.xvg", package = "xvm"))
# Export as TSV
export_xvg(xvg, "rmsd.tsv", sep = "\t")
# Export as CSV
export_xvg(xvg, "rmsd.csv", sep = ",")

## End(Not run)
```

`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
```

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,
  merge = FALSE,
  title = NULL,
  subtitle = NULL,
  use_color_scale = NULL,
  ...
)
```

Arguments

xvg_data	xvg data object returned by read_xvg
merge	logical; if TRUE and multiple datasets provided, merge them (default: FALSE)
title	chart title (default uses xvg file's title)
subtitle	chart subtitle (default uses xvg file's subtitle)
use_color_scale	custom color scale function (e.g., ggsci::scale_color_bmj) to override default colors
...	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)
```

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)
```

summary_xvg *summarize xvg data compute basic summary statistics (mean, sd, min, median, max) for each variable in one or more xvg_data objects.*

Description

summarize xvg data compute basic summary statistics (mean, sd, min, median, max) for each variable in one or more xvg_data objects.

Usage

```
summary_xvg(xvg_data, merge_results = FALSE)
```

Arguments

`xvg_data`	a list of class 'xvg_data' or a list containing multiple 'xvg_data' objects, as returned by `read_xvg()`.
`merge_results`	logical, whether to combine results from multiple objects (default: FALSE). When TRUE, results will include a 'group' column identifying the source.

Value

a data.frame with columns:

group (Optional) Source identifier when processing multiple objects with merge_results=TRUE.

variable Name of the variable (column) in the xvg data.

mean Arithmetic mean of that variable.

sd Standard deviation.

min Minimum value.

median Median value.

max Maximum value.

Examples

```
path <- system.file("extdata/rmsd.xvg", package = "xvm")
xvg_data <- read_xvg(path)
summary_xvg(xvg_data)
```

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