

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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export_xvg	<i>export xvg data object</i>
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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

<code>xvg_data</code>	An object of class <code>xvg_data</code> , or a list of <code>xvg_data</code> objects, as returned by <code>read_xvg()</code> .
<code>file</code>	Path to the output file (any extension is acceptable).
<code>sep</code>	Field separator (e.g., <code>"\t"</code> for TSV, <code>","</code> for CSV). Default is <code>"\t"</code> .
<code>row.names</code>	Logical, whether to write row names. Default is <code>FALSE</code> .
<code>merge</code>	Logical, whether to merge multiple <code>xvg_data</code> objects before exporting. Default is <code>FALSE</code> .
<code>...</code>	Additional arguments passed to <code>write.table()</code> .

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	<i>plot xpm data</i>
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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	<i>generate 3d scatter plot from xpm data</i>
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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	<i>generate faceted plots from xpm data</i>
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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

<code>xvg_data</code>	xvg data object returned by <code>read_xvg</code>
<code>merge</code>	logical; if TRUE and multiple datasets provided, merge them (default: FALSE)
<code>title</code>	chart title (default uses xvg file's title)
<code>subtitle</code>	chart subtitle (default uses xvg file's subtitle)
<code>use_color_scale</code>	custom color scale function (e.g., <code>ggsci::scale_color_bmj</code>) to override default colors
<code>...</code>	additional parameters passed to <code>ggplot2::geom_line</code>

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