

mm_trj
V.1.1.1

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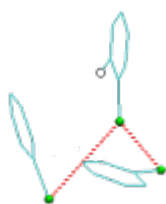
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Chapter 1

mm_trj



1.1 Introduction

About this program:

- Program that generates trajectory files

Developer:

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License:

- GPL

1.2 How to use

Usage:

```
mm_trj -i INPUT_TRJ -t INPUT_TYPE -s NUMBER -a INPUT_ATOMS -o OUTPUT [ -tt TOTAL_TYPES ]  
                                           [ -l LOGFILE ] [ -q ] [ -h ]
```

Parameters:

-i	- input file name
-t	- type of trajectory. Supported formats: gmx, puma
-s	- number of trajectory steps (integer)
-a	- input file with atom types. See file format in manual
-o	- mask of output files
-tt	- number of different atom types. Default is 1024
-l	- log enable
-q	- quiet enable
-h	- show this help and exit

Chapter 2

Install

2.1 Requirements

The application mm_trj requires the following external stuff:

- cmake \geq 2.8
- gcc \geq 4.8

2.2 How to install

2.2.1 Linux

```
* mkdir build && cd build
* cmake -DCMAKE_INSTALL_PREFIX=/usr -DCMAKE_BUILD_TYPE=Release ../
* make
* make install
*
```

2.2.2 Windows

```
* create project file using 'cmake'
* compile project
*
```

You may also download compiled executable file for Win_x86.

Chapter 3

Changelog

V.1.1.1 (2013-09-03)

- optimization

V.1.1.0 (2013-09-02)

- added help window
- added help docs
- small bug fixes

V.1.0.3 (2013-08-30)

- bug fixes

V.1.0.1 (2013-07-27)

- initial release

Chapter 4

File Index

4.1 File List

Here is a list of all files with brief descriptions:

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Chapter 5

File Documentation

5.1 src/add_main.c File Reference

```
#include <stdio.h>
#include "messages.h"
```

Functions

- int [error_checking](#) (const char *input, const char *input_at, const char *output, const int step, const int type)
function that checks errors in input variables
- int [print_message](#) (const int quiet, FILE *std_output, const int log, FILE *f_log, const int mode, const char *str)
function that prints message in log and stdout
- int [set_defaults](#) (char *input, char *input_at, int *log, char *output, int *step, int *total_types, int *type, int *quiet)
function that sets default values of variables

5.1.1 Function Documentation

5.1.1.1 int error_checking (const char * input, const char * input_at, const char * output, const int step, const int type)

function that checks errors in input variables

```
* error\_checking (cell, from, input, num_needed_at, needed_at, output, to);
*
```

Parameters

<i>input</i>	input file name
<i>input_at</i>	input file name with atom types
<i>output</i>	output file name
<i>step</i>	number of trajectory steps
<i>type</i>	type of trajectory

Returns

- 11 - error in 'input_at'
- 12 - error in 'input'
- 13 - error in 'output'
- 14 - error in 'step'
- 15 - error in 'type'
- 0 - exit without errors

5.1.1.2 `int print_message (const int quiet, FILE * std_output, const int log, FILE * f_log, const int mode, const char * str)`

function that prints message in log and stdout

```
* print_message (quiet, stdout, log, f_log, 0, str);
*
```

Parameters

<i>quiet</i>	status of quiet-mode
<i>std_output</i>	stdout
<i>log</i>	status of log-mode
<i>f_log</i>	log file
<i>mode</i>	number of message in "messages.c"
<i>str</i>	additional text in message

Returns

- 0 - exit without errors

5.1.1.3 `int set_defaults (char * input, char * input_at, int * log, char * output, int * step, int * total_types, int * type, int * quiet)`

function that sets default values of variables

```
* set_defaults (input, input_at, &log, output, &step, &type, &quiet);
*
```

Parameters

<i>input</i>	input file name
<i>input_at</i>	input file name with atom types
<i>log</i>	status of log-mode
<i>output</i>	output file name
<i>step</i>	number of trajectory steps
<i>total_types</i>	number of different atom types
<i>type</i>	type of trajectory
<i>quiet</i>	status of quiet-mode

Returns

- 0 - exit without errors

5.2 src/atom_types.c File Reference

```
#include <stdio.h>
```

Functions

- int [reading_atoms](#) (const char *input_at, int *num_types, int *num_mol, int *num_atoms, char *ch_atom_types, int *atom_types, const int total_types)
function that reads atom types from input file

5.2.1 Function Documentation

5.2.1.1 int [reading_atoms](#) (const char * *input_at*, int * *num_types*, int * *num_mol*, int * *num_atoms*, char * *ch_atom_types*, int * *atom_types*, const int *total_types*)

function that reads atom types from input file

```
* reading\_atoms (input_at, &num_types, num_mol, num_atoms, ch_atom_types, atom_types,
*                 total_types);
*
```

Parameters

<i>input_at</i>	input file name with atom types
<i>num_types</i>	number of molecule types
<i>num_mol</i>	massive of number of molecules of selected type
<i>num_atoms</i>	massive of number of atoms of selected molecule
<i>ch_atom_types</i>	massive of char atom types
<i>atom_types</i>	massive of atom types
<i>total_types</i>	number of different atom types

Returns

- 1 - error in opening file
- 2 - error in file format
- 3 - memory error
- 0 - exit without errors

5.3 src/main.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include "add_main.h"
#include "atom_types.h"
#include "messages.h"
#include "print_trj.h"
#include "read_gmx.h"
#include "read_puma.h"
```

Functions

- int [main](#) (int argc, char *argv[])

5.3.1 Function Documentation

5.3.1.1 int [main](#) (int *argc*, char * *argv*[])

Returns

- 1 - error in error_checking
- 2 - input file does not exist
- 3 - memory error
- 4 - unknown flag
- 0 - exit without errors

5.4 src/messages.c File Reference

```
#include <stdio.h>
#include <time.h>
```

Functions

- int [message](#) (const int log, const int mode, const char *text, FILE *output)
function that prints messages to output

5.4.1 Function Documentation

5.4.1.1 int [message](#) (const int *log*, const int *mode*, const char * *text*, FILE * *output*)

function that prints messages to output

```
* message (log, mode, text, output);
*
```

Parameters

<i>log</i>	equal to 1 if print to logfile
<i>mode</i>	number of message
<i>text</i>	additional text
<i>output</i>	output file (may be stdout)

Returns

- 1 - unknown mode
- 0 - exit without errors

5.5 src/print_trj.c File Reference

```
#include <stdio.h>
```

Functions

- int [printing_trj](#) (const char *filename, const int atoms, const int num_types, const int *num_mol, const int *num_atoms, const char *ch_atom_types, const int *atom_types, const float *coords)
function that prints trajectory snapshots

5.5.1 Function Documentation

5.5.1.1 `int printing_trj (const char * filename, const int atoms, const int num_types, const int * num_mol, const int * num_atoms, const char * ch_atom_types, const int * atom_types, const float * coords)`

function that prints trajectory snapshots

```
* printing_trj (filename, atoms, num_types, num_mol, num_atoms, ch_atom_types,
*               atom_types, coords);
*
```

Parameters

<i>filename</i>	output file name
<i>atoms</i>	number of atoms in system
<i>num_types</i>	number of molecule types
<i>num_mol</i>	massive of number of molecule of selected type
<i>num_atoms</i>	massive of number of atoms of selected molecule
<i>ch_atom_types</i>	massive of char atom types
<i>atom_types</i>	massive of atom types
<i>coords</i>	massive of coordinates

Returns

0 - exit without errors

5.6 src/read_gmx.c File Reference

```
#include <math.h>
#include <stdio.h>
#include "print_trj.h"
```

Functions

- `int translate_coords (const float coords, const float cell, float *trans)`
function that translates coordinate
- `int rw_gmx (const char *input, const int step, const char *output, const int num_types, const int *num_mol, const int *num_atoms, const char *ch_atom_types, const int *atom_types, float *coords)`
function that read GROMACS trajectory file and write to output

5.6.1 Function Documentation

5.6.1.1 `int rw_gmx (const char * input, const int step, const char * output, const int num_types, const int * num_mol, const int * num_atoms, const char * ch_atom_types, const int * atom_types, float * coords)`

function that read GROMACS trajectory file and write to output

```
* rw_gmx (input, step, output, num_types, num_mol, num_atoms, ch_atom_types,
*         atom_types, coords);
*
```

Parameters

<i>input</i>	input file name
<i>step</i>	number of trajectory steps
<i>output</i>	mask of output files
<i>num_types</i>	number of molecule types
<i>num_mol</i>	massive of number of molecule of selected type
<i>num_atoms</i>	massive of number of atoms of selected molecule
<i>ch_atom_types</i>	massive of char atom types
<i>atom_types</i>	massive of atom types
<i>coords</i>	massive of coordinates

Returns

- 1 - file does not exist
- 0 - exit without errors

5.6.1.2 int translate_coords (const float *coords*, const float *cell*, float * *trans*)

function that translates coordinate

```
* translate_coords (coords[3*i+j], cell[j], trans);
*
```

Parameters

<i>coords</i>	coordinate
<i>cell</i>	cell size
<i>trans</i>	massive of translated coordinates

Returns

- 0 - exit without errors

5.7 src/read_puma.c File Reference

```
#include <stdio.h>
#include "print_trj.h"
```

Functions

- int [rw_puma](#) (const char **input*, const int *step*, const char **output*, const int *num_types*, const int **num_mol*, const int **num_atoms*, const char **ch_atom_types*, const int **atom_types*, float **coords*)
function that read PUMA trajectory file and write to output

5.7.1 Function Documentation

5.7.1.1 int rw_puma (const char * *input*, const int *step*, const char * *output*, const int *num_types*, const int * *num_mol*, const int * *num_atoms*, const char * *ch_atom_types*, const int * *atom_types*, float * *coords*)

function that read PUMA trajectory file and write to output

```
* rw_puma (input, step, output, num_types, num_mol, num_atoms, ch_atom_types,
*          atom_types, coords);
*
```

Parameters

<i>input</i>	input file name
<i>step</i>	number of trajectory steps
<i>output</i>	mask of output files
<i>num_types</i>	number of molecule types
<i>num_mol</i>	massive of number of molecule of selected type
<i>num_atoms</i>	massive of number of atoms of selected molecule
<i>ch_atom_types</i>	massive of char atom types
<i>atom_types</i>	massive of atom types
<i>coords</i>	massive of coordinates

Returns

- 1 - file does not exist
- 0 - exit without errors

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