

Fluid Simulation

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Chapter 1

Hierarchical Index

1.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

particle_parameter	28
box	10
brown_factor	12
fluctuation	16
initialization	22
BD_simulation	8
fluid_simulation	18
MD_simulation	24
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cell_list	14
force	20
initialization	22
force	20
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initialization	22
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Chapter 2

Class Index

2.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

BD_simulation	8
box	10
brown_factor	12
cell_list	14
fluctuation	16
fluid_simulation	18
force	20
initialization	22
MD_simulation	24
output	26
particle_parameter	28
position	30
time_step	32
velocity	34

Chapter 3

File Index

3.1 File List

Here is a list of all documented files with brief descriptions:

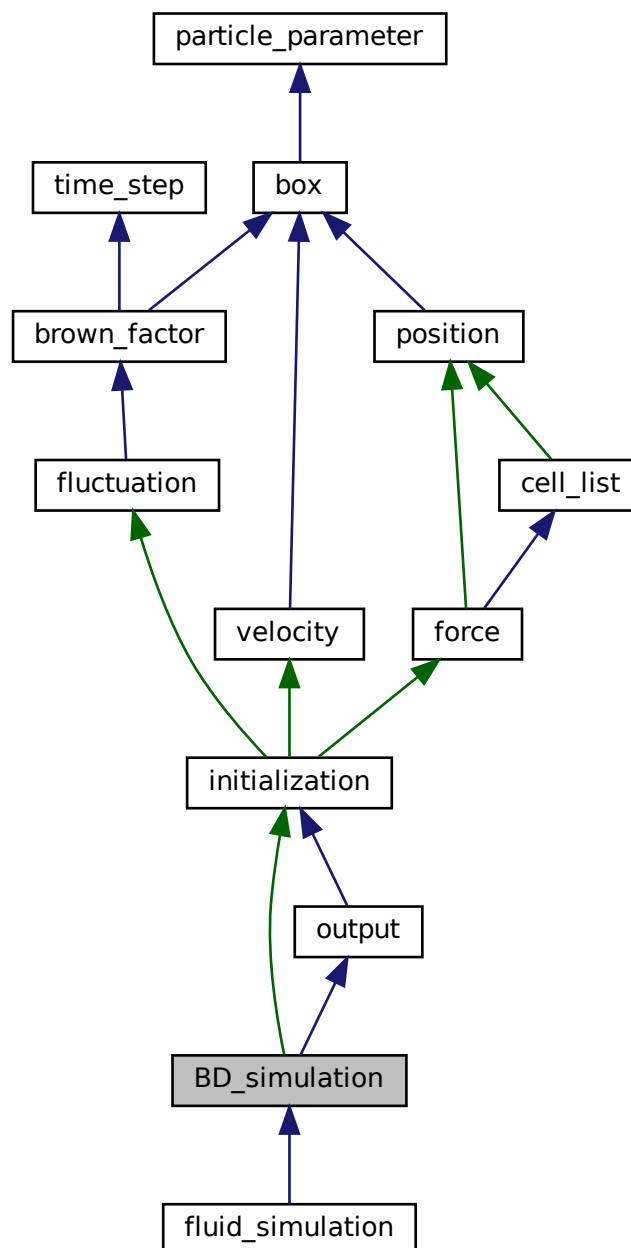
include/fluid_simulation.hpp	37
include/main.hpp	54
include/implementation/BD_simulation.hpp	??
include/implementation/cell_list.hpp	38
include/implementation/fluctuation.hpp	40
include/implementation/force.hpp	42
include/implementation/implementation.hpp	??
include/implementation/MD_simulation.hpp	??
include/implementation/position.hpp	44
include/implementation/velocity.hpp	46
include/initialization/box.hpp	48
include/initialization/brown_factor.hpp	49
include/initialization/initialization.hpp	??
include/initialization/particle_parameter.hpp	51
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src/fluid_simulation.cpp	56
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src/initialization/box.cpp	63
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src/initialization/particle_parameter.cpp	66
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Chapter 4

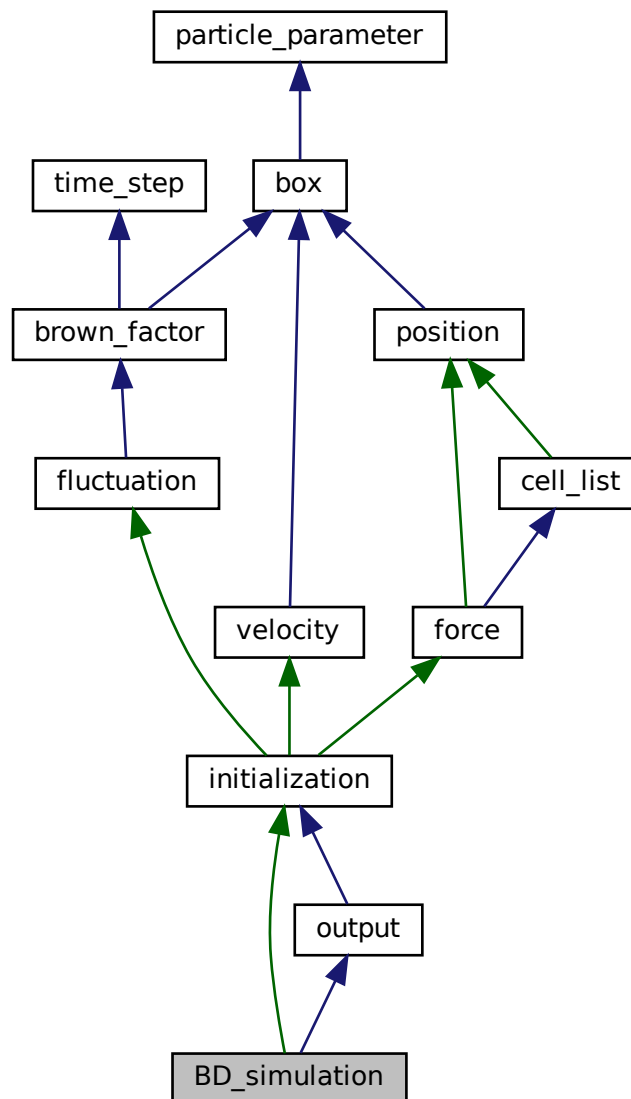
Class Documentation

4.1 BD_simulation Class Reference

Inheritance diagram for BD_simulation:



Collaboration diagram for BD_simulation:



Public Member Functions

- void **BD_relaxation** ()
- void **BD_implementation** ()

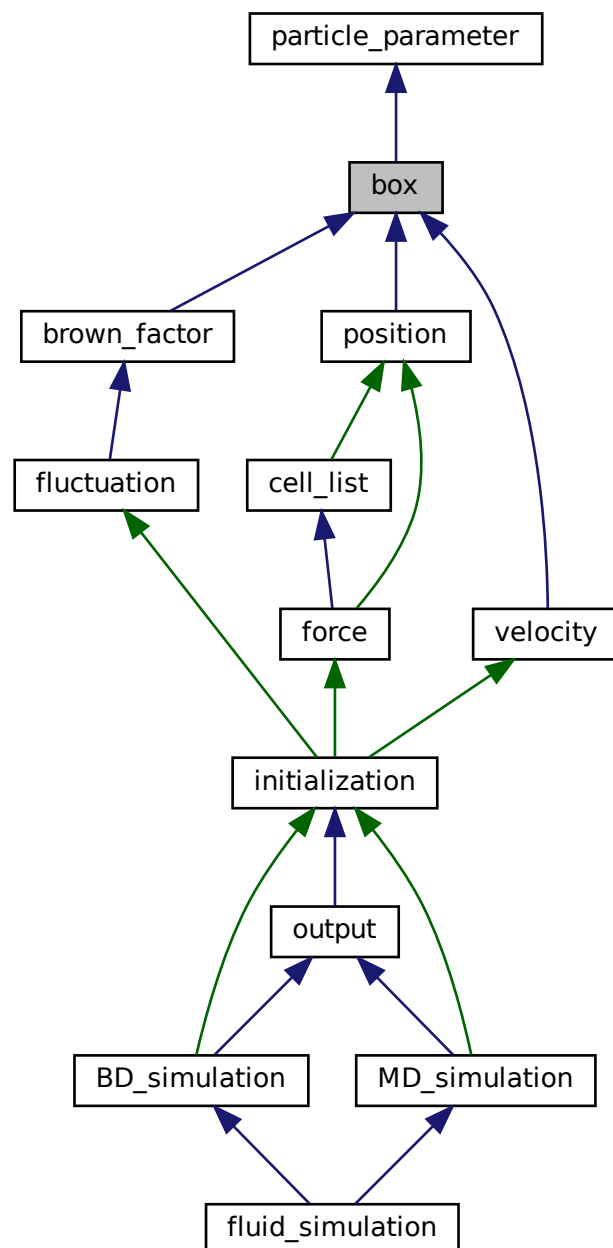
Additional Inherited Members

The documentation for this class was generated from the following files:

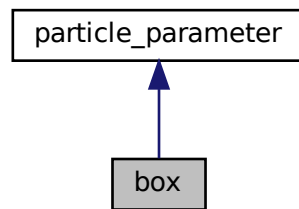
- include/implementation/BD_simulation.hpp
- src/implementation/[BD_simulation.cpp](#)

4.2 box Class Reference

Inheritance diagram for box:



Collaboration diagram for box:



Public Member Functions

- void **kT** (const double input)
- double **kT** () const
- void **l_b** (const int ax, const double input)
 - set the periodic boundary condition*
- std::array< double, 3 > **l_b** () const
- std::array< double, 3 > **half_l_b** () const
- std::array< double, 3 > **inv_l_b** () const
- void **Nm** (const uint64_t input)
- void **density** (const double input)
- uint64_t **Nm** () const
- void **calc_Nm** ()
- void **calc_density** ()
- double **density** () const
- double **real_density** () const

4.2.1 Member Function Documentation

4.2.1.1 l_b()

```

void box::l_b (
    const int ax,
    const double input )

```

set the periodic boundary condition

Parameters

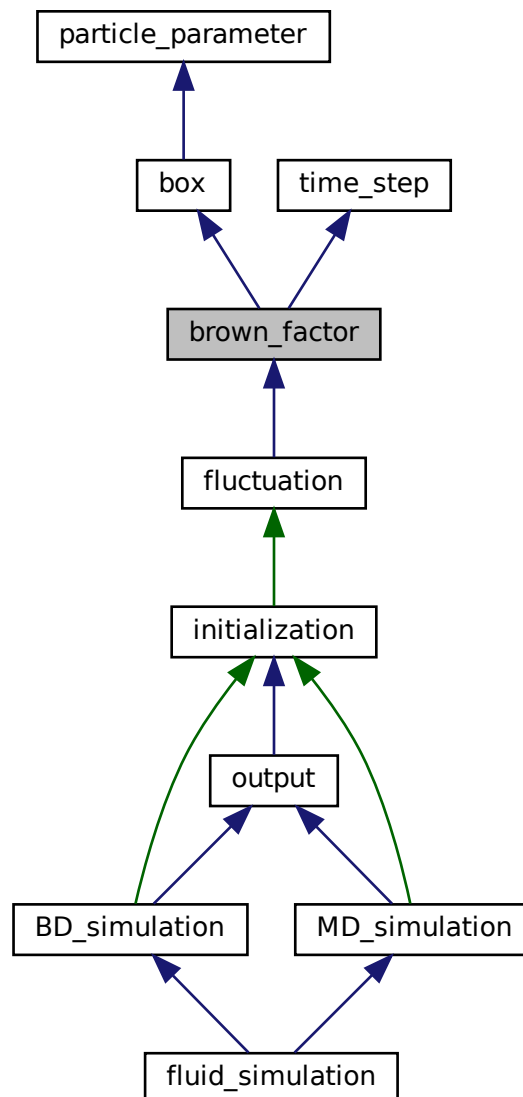
$l_b \leftarrow$	
$_x$	
$l_b \leftarrow$	
$_y$	
$l_b \leftarrow$	
$_z$	

The documentation for this class was generated from the following files:

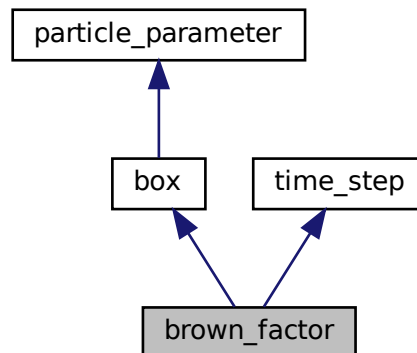
- [include/initialization/box.hpp](#)
- [src/initialization/box.cpp](#)

4.3 brown_factor Class Reference

Inheritance diagram for brown_factor:



Collaboration diagram for brown_factor:



Public Member Functions

- void **calc_BD_factor** ()
- double **BD_r_1** () const
- double **BD_r_2** () const
- double **BD_v_1** () const
- double **BD_v_2** () const
- double **BD_v_3** () const
- double **BD_g0_1** () const
- double **BD_g1_1** () const
- double **BD_g1_2** () const

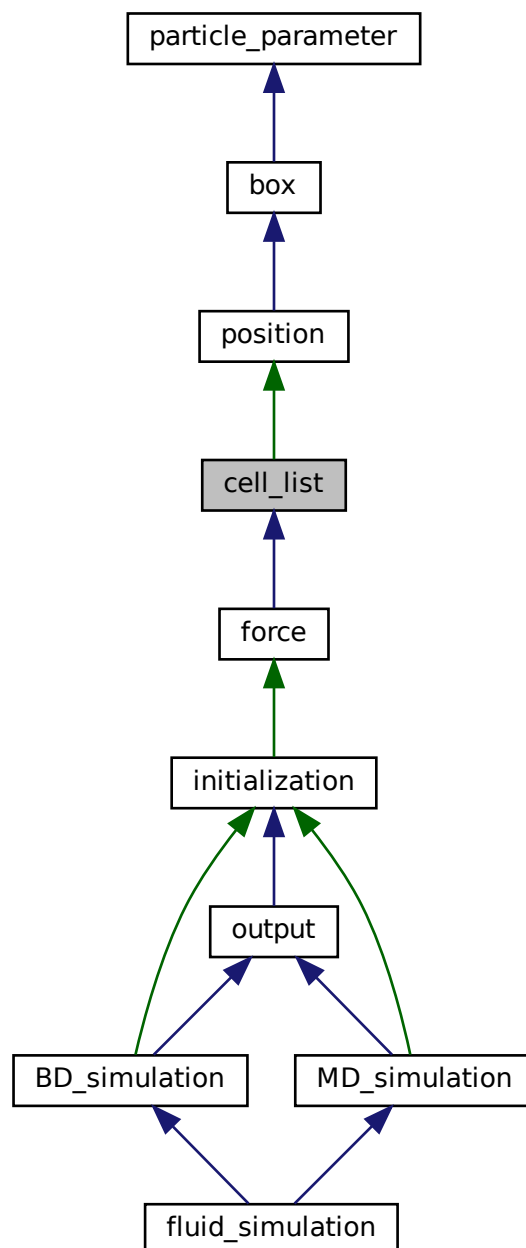
Additional Inherited Members

The documentation for this class was generated from the following files:

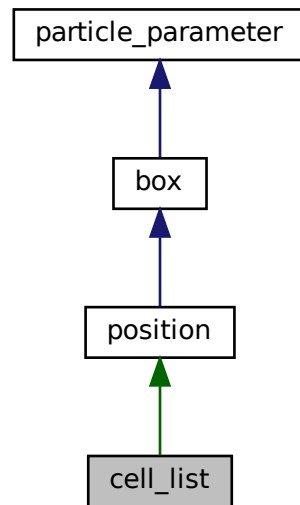
- include/initialization/[brown_factor.hpp](#)
- src/initialization/[brown_factor.cpp](#)

4.4 cell_list Class Reference

Inheritance diagram for cell_list:



Collaboration diagram for cell_list:



Public Member Functions

- void `init_cell_list` (const double &cell_size)
- void `refresh_cell_list` ()

Public Attributes

- std::vector< std::vector< uint64_t > > `cell_list_ij`

Additional Inherited Members

4.4.1 Member Function Documentation

4.4.1.1 `init_cell_list()`

```
void cell_list::init_cell_list (
    const double & cell_size )
```

calculate the number and length of cell

generate empty cell

generate cell list of i-j paar

4.4.1.2 refresh_cell_list()

```
void cell_list::refresh_cell_list ( )
```

clear all the cell in the list

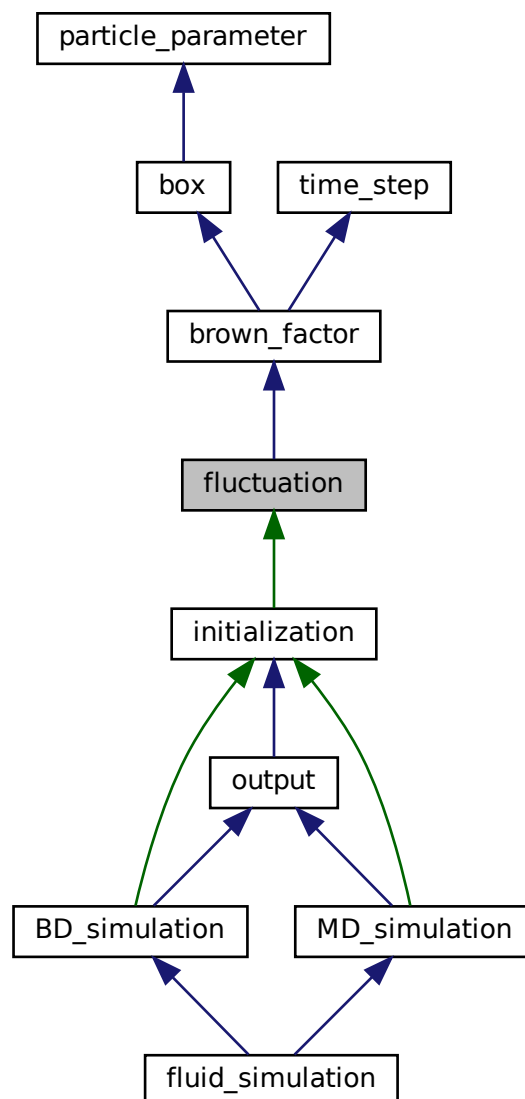
put the index in the cell list

The documentation for this class was generated from the following files:

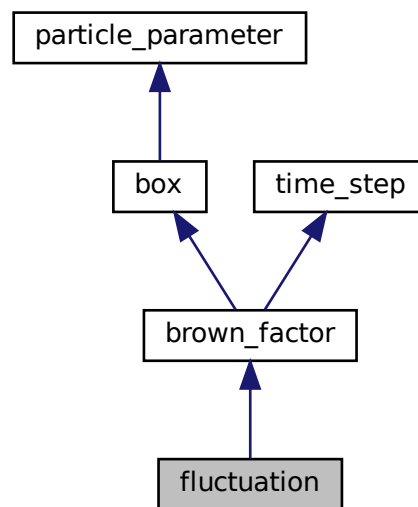
- include/implementation/[cell_list.hpp](#)
- src/implementation/[cell_list.cpp](#)

4.5 fluctuation Class Reference

Inheritance diagram for fluctuation:



Collaboration diagram for fluctuation:



Public Member Functions

- void `init_fluctuation` ()
- void `generate_Gamma` ()

Protected Attributes

- `std::vector< std::array< double, 3 > > g0`
- `std::vector< std::array< double, 3 > > g1`

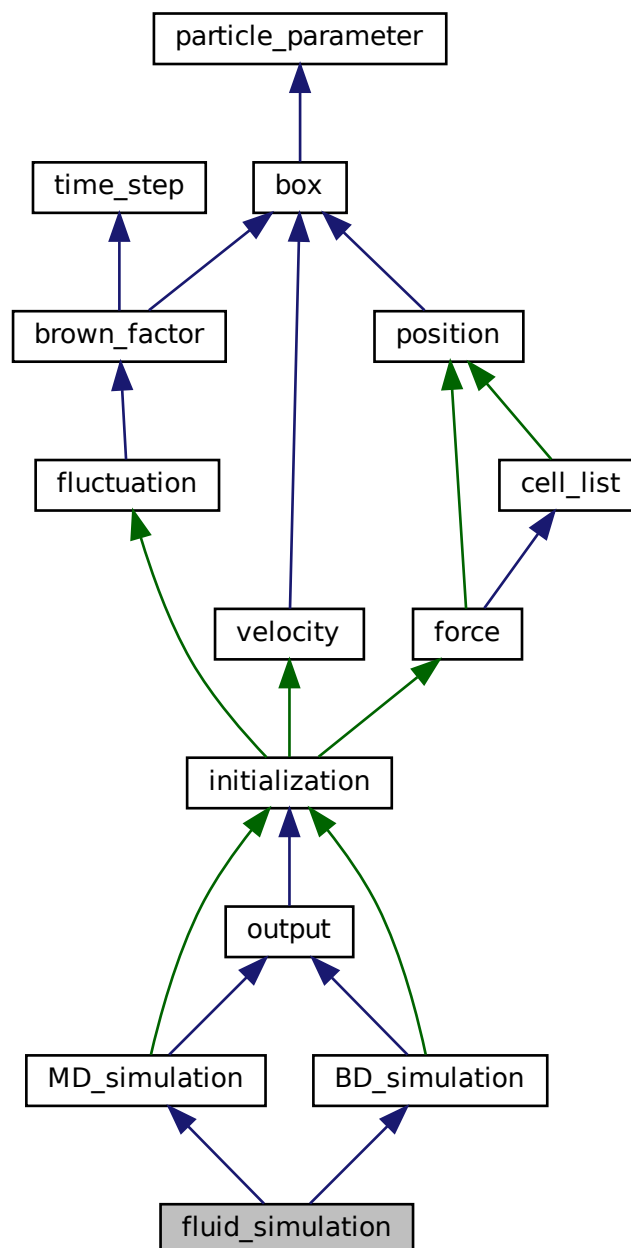
Additional Inherited Members

The documentation for this class was generated from the following files:

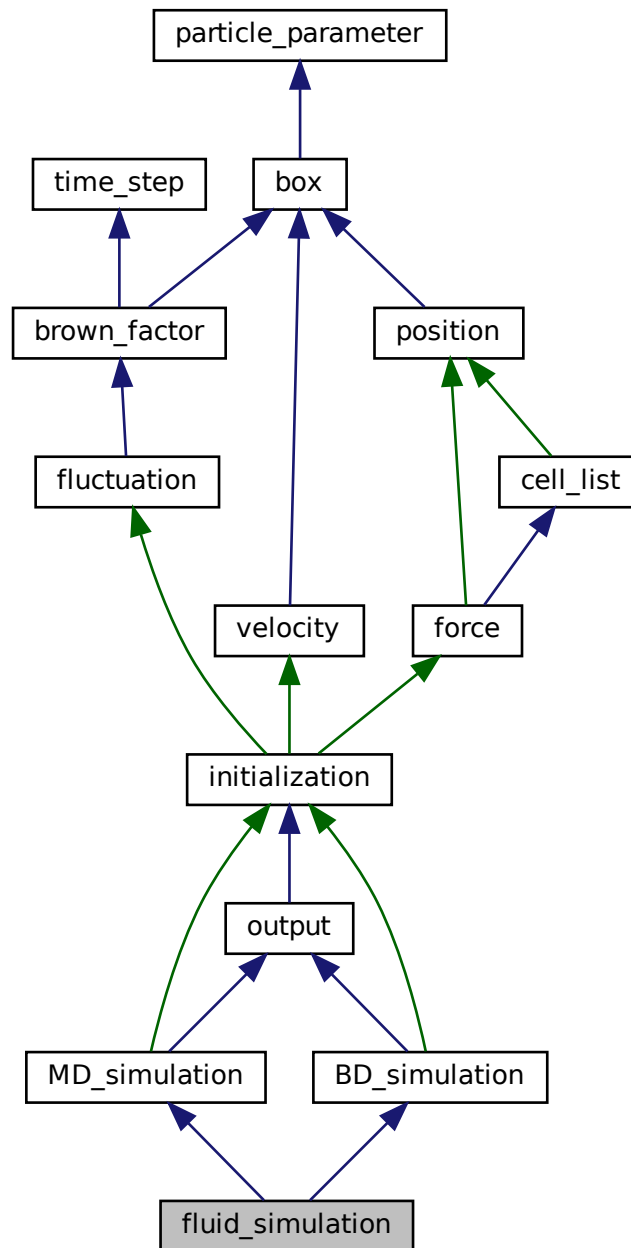
- [include/implementation/fluctuation.hpp](#)
- [src/implementation/fluctuation.cpp](#)

4.6 fluid_simulation Class Reference

Inheritance diagram for fluid_simulation:



Collaboration diagram for fluid_simulation:



Public Member Functions

- **fluid_simulation** (const int argc, const char **argv)
- void **relax** ()
- void **implement** ()

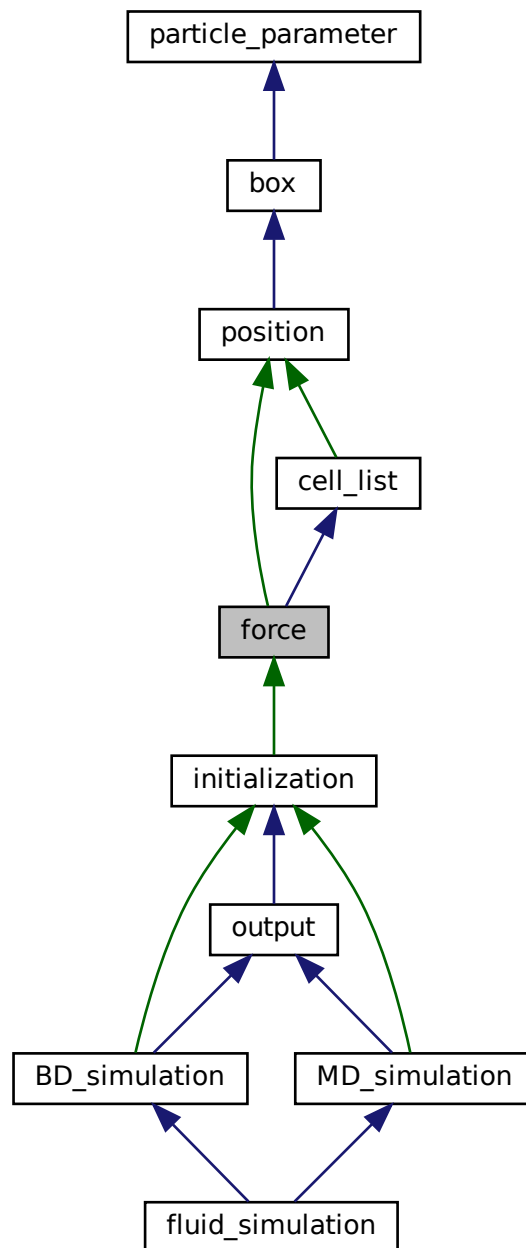
Additional Inherited Members

The documentation for this class was generated from the following files:

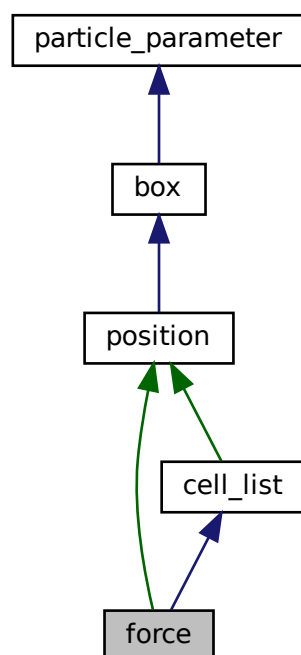
- [include/fluid_simulation.hpp](#)
- [src/fluid_simulation.cpp](#)

4.7 force Class Reference

Inheritance diagram for force:



Collaboration diagram for force:



Public Member Functions

- void **init_force** ()
- void **calc_force** ()
- double **E_pot** () const

Protected Attributes

- std::vector< std::array< double, 3 > > **f0**
- std::vector< std::array< double, 3 > > **f1**

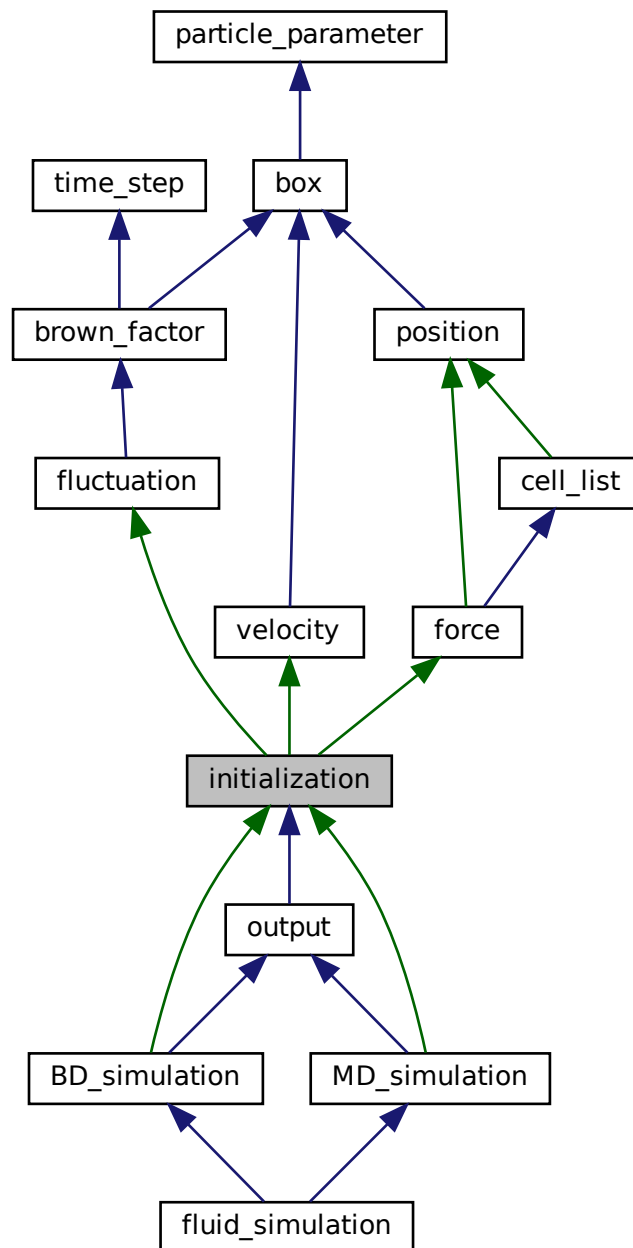
Additional Inherited Members

The documentation for this class was generated from the following files:

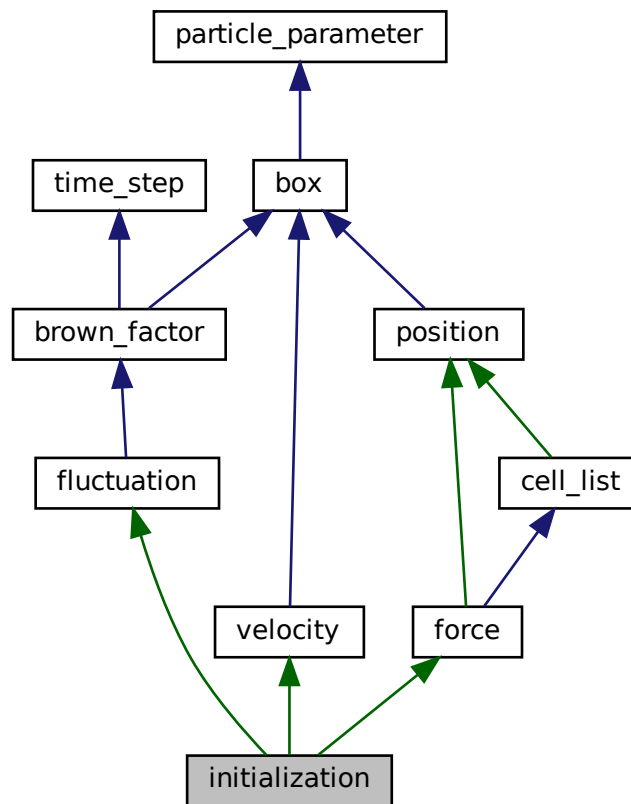
- include/implementation/[force.hpp](#)
- src/implementation/[force.cpp](#)

4.8 initialization Class Reference

Inheritance diagram for initialization:



Collaboration diagram for initialization:



Public Member Functions

- void **init** (const int argc, const char **argv)
- void **read_arg** (const int argc, const char **argv)
- void **read_config** ()

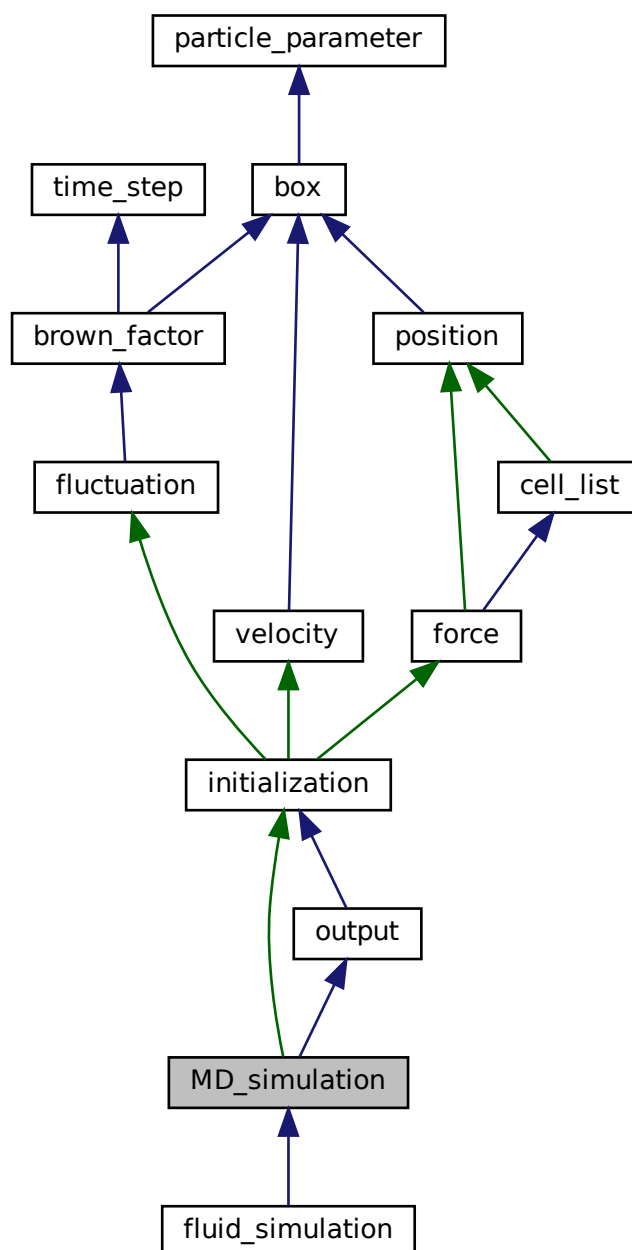
Additional Inherited Members

The documentation for this class was generated from the following files:

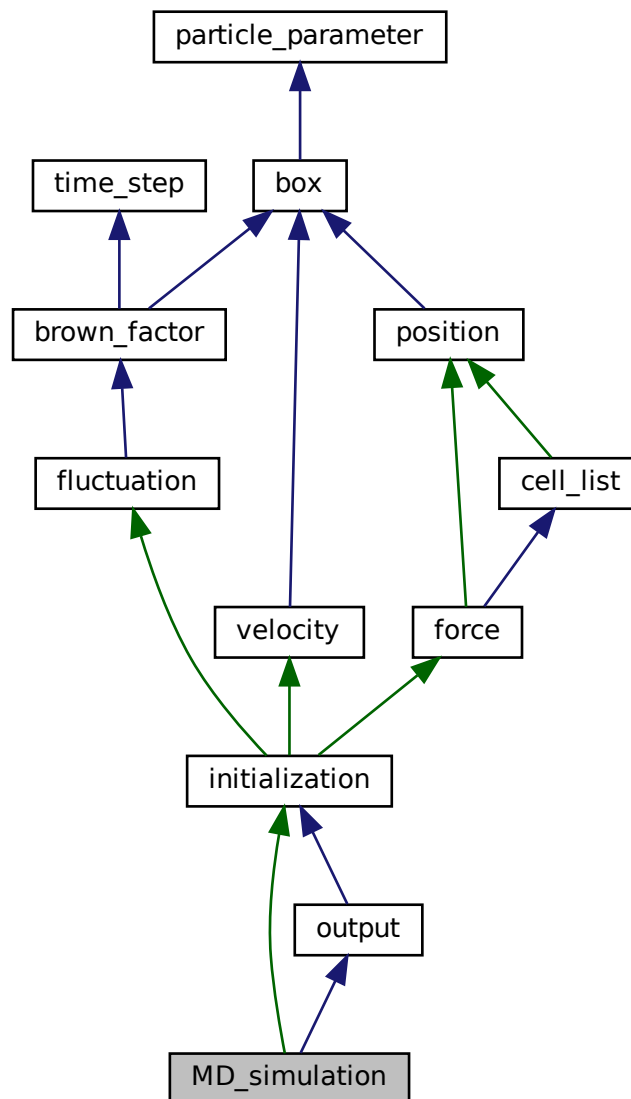
- include/initialization/initialization.hpp
- src/initialization/initialization.cpp

4.9 MD_simulation Class Reference

Inheritance diagram for MD_simulation:



Collaboration diagram for MD_simulation:



Public Member Functions

- void **MD_relaxation** ()
- void **MD_implementation** ()

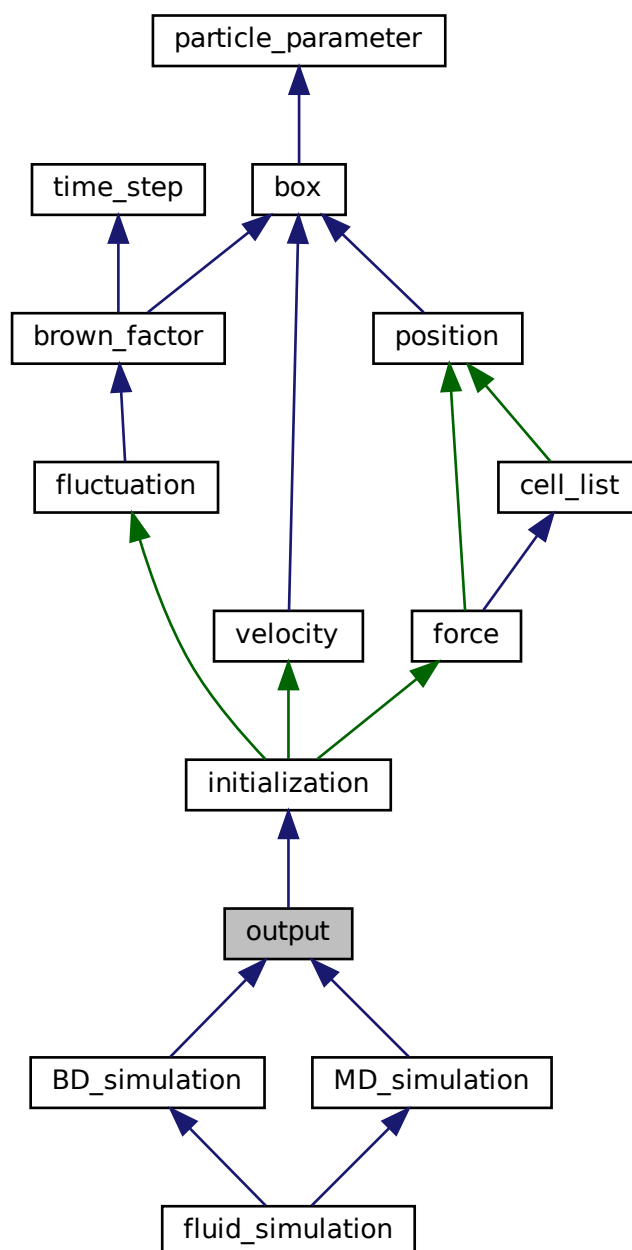
Additional Inherited Members

The documentation for this class was generated from the following files:

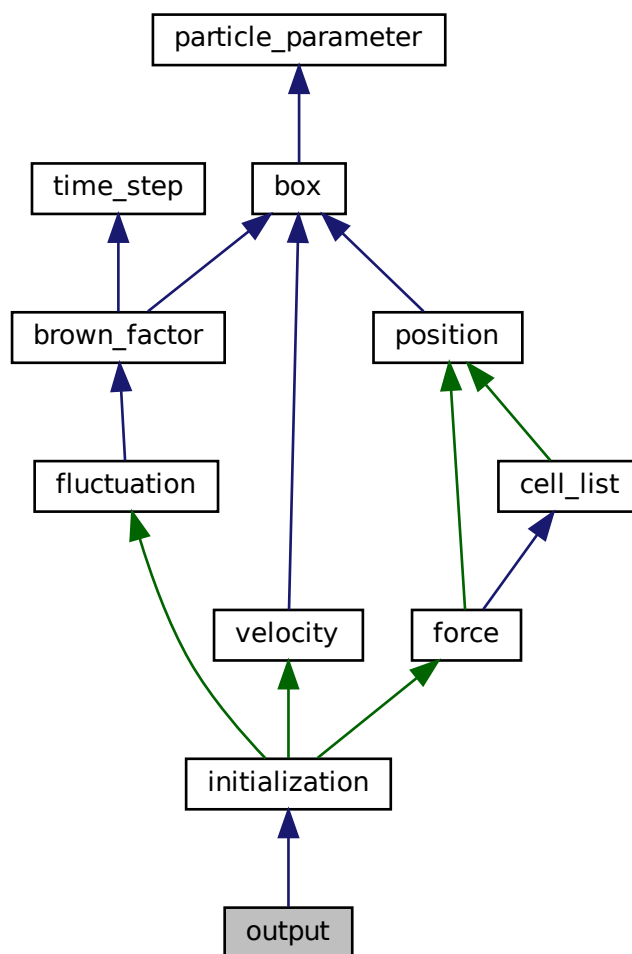
- include/implementation/MD_simulation.hpp
- src/implementation/MD_simulation.cpp

4.10 output Class Reference

Inheritance diagram for output:



Collaboration diagram for output:



Public Member Functions

- void **print_energy** ()
- void **write_cfg** ()
- void **write_energy** ()
- void **write_last_cfg** ()

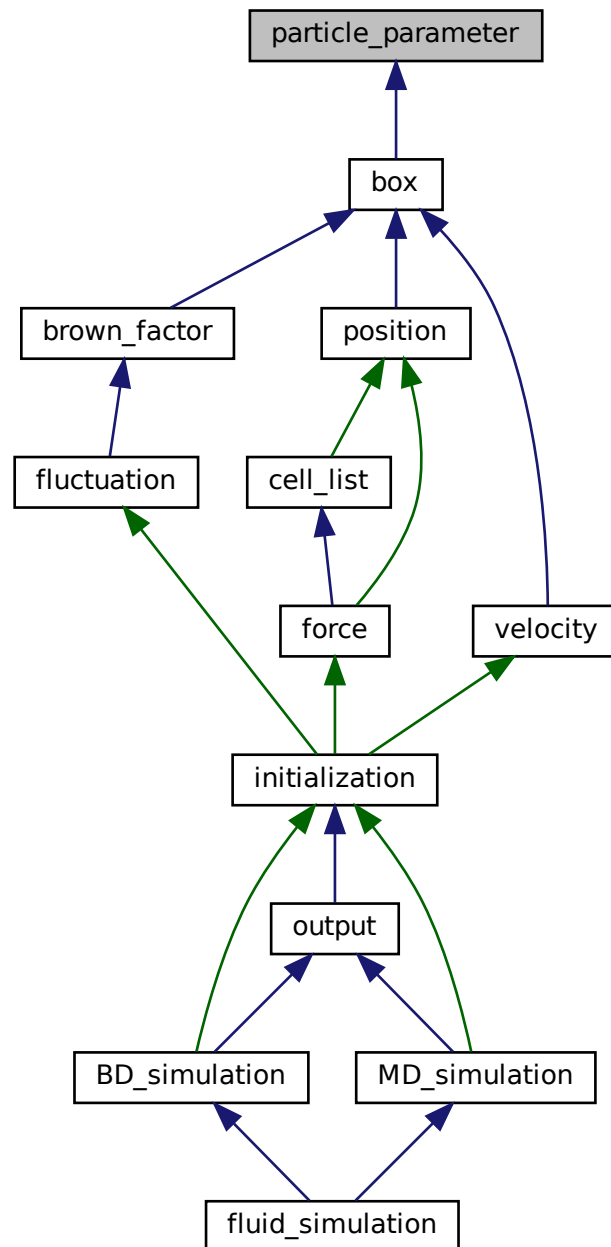
Additional Inherited Members

The documentation for this class was generated from the following files:

- [include/output/output.hpp](#)
- [src/output/output.cpp](#)

4.11 particle_parameter Class Reference

Inheritance diagram for particle_parameter:



Public Member Functions

- void **m** (const double input)
- double **m** () const

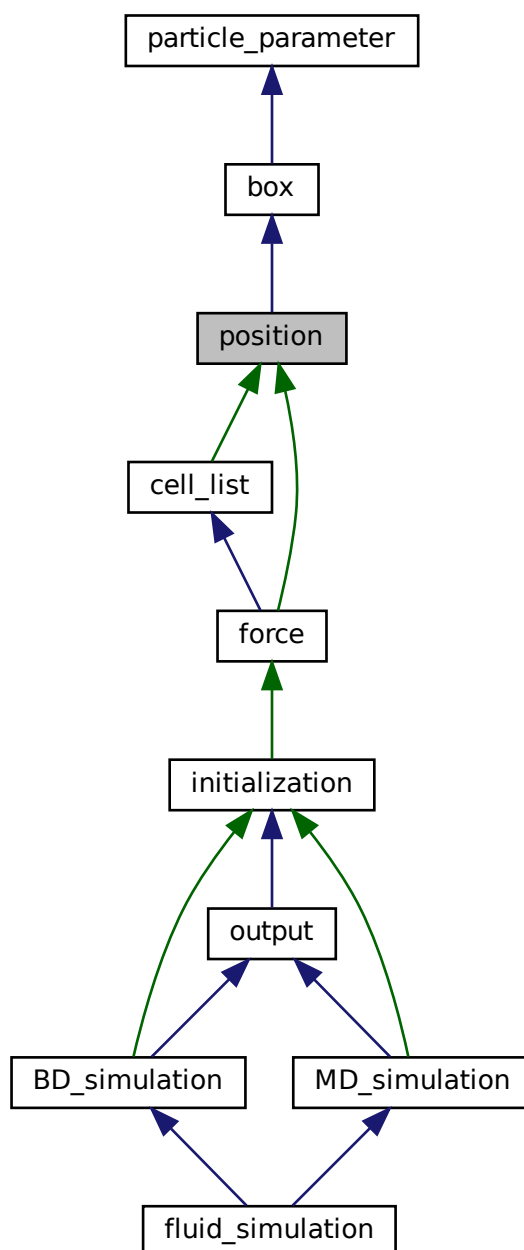
- void **gamma** (const double input)
- double **gamma** () const
- void **epsilon** (const double input)
- double **epsilon** () const
- void **sigma** (const double input)
- double **sigma** () const
- double **r2_cut** () const
- double **sig2** () const

The documentation for this class was generated from the following files:

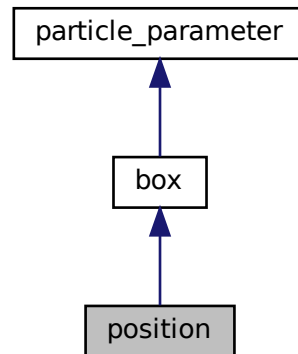
- include/initialization/[particle_parameter.hpp](#)
- src/initialization/[particle_parameter.cpp](#)

4.12 position Class Reference

Inheritance diagram for position:



Collaboration diagram for position:



Public Member Functions

- void **init_position** ()
- double **r_in_box** (const uint64_t &i, const int &ax)
- double **minium_image** (const uint64_t &i, const uint64_t &j, const int &ax)

Protected Attributes

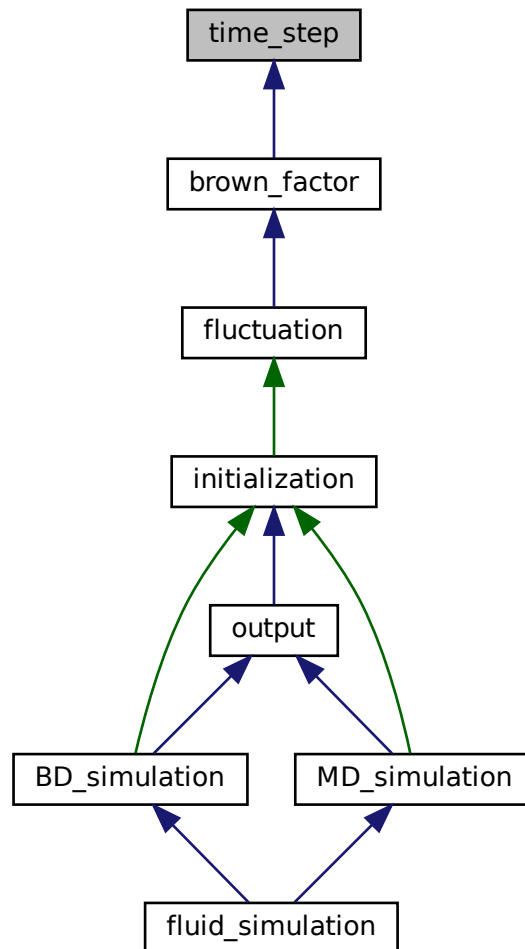
- std::vector< std::array< double, 3 > > **r**
- std::vector< std::array< double, 3 > > **dr**

The documentation for this class was generated from the following files:

- include/implementation/[position.hpp](#)
- src/implementation/[position.cpp](#)

4.13 time_step Class Reference

Inheritance diagram for time_step:



Public Member Functions

- void **MD_Steps** (const double input)
 - void **Relax_time** (const uint64_t input)
 - void **MD_time** (const double input)
 - void **h** (const double input)
 - uint64_t **MD_Steps** () const
 - uint64_t **Relax_Steps** () const
 - double **MD_time** () const
 - double **step_time** () const
 - double **h** () const
 - double **half_h** () const
- out put time step h*

out put half time step

- double **half_h2** () const
- uint64_t **time_0001** () const
- uint64_t **time_001** () const
- uint64_t **time_01** () const
- uint64_t **time_1** () const
- uint64_t **time_10** () const
- uint64_t **time_100** () const
- uint64_t **time_1000** () const

Public Attributes

- uint64_t **step**

4.13.1 Member Function Documentation

4.13.1.1 h()

```
double time_step::h ( ) const
```

out put time step h

Returns

double

4.13.1.2 half_h()

```
double time_step::half_h ( ) const
```

out put half time step

Returns

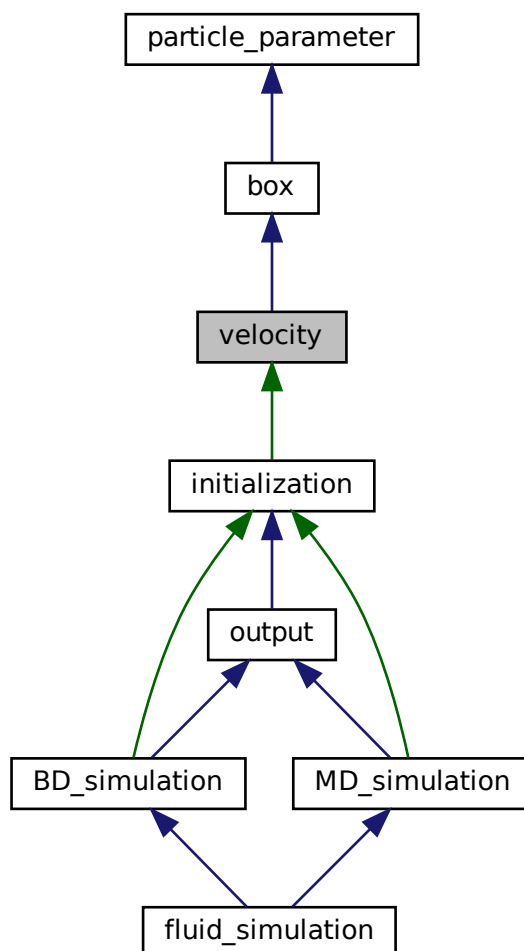
double

The documentation for this class was generated from the following files:

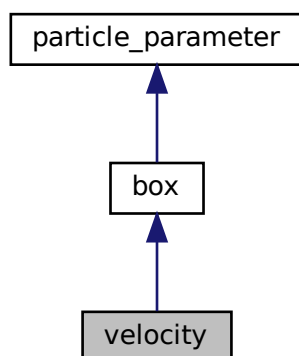
- include/initialization/[time_step.hpp](#)
- src/initialization/[time_step.cpp](#)

4.14 velocity Class Reference

Inheritance diagram for velocity:



Collaboration diagram for velocity:



Public Member Functions

- void **init_velocity** ()
- void **vel_correcter** ()
- void **calc_E_kin** ()
- double **E_kin** () const

Protected Attributes

- `std::vector< std::array< double, 3 > > v`

The documentation for this class was generated from the following files:

- `include/implementation/velocity.hpp`
- `src/implementation/velocity.cpp`

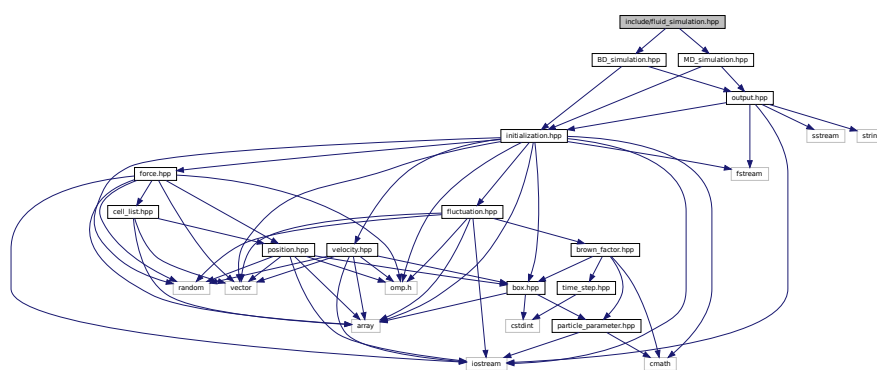
File Documentation

5.1 include/fluid_simulation.hpp File Reference

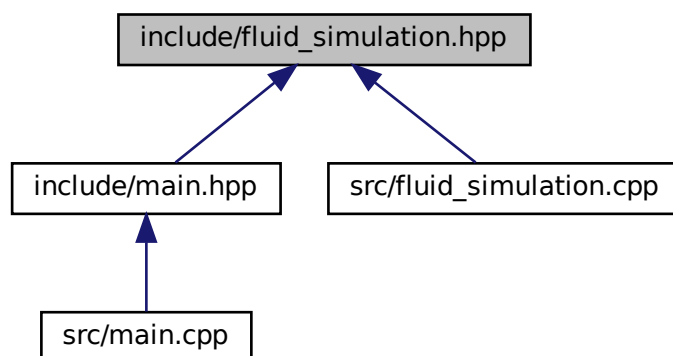
```
#include "BD_simulation.hpp"
```

```
#include "MD_simulation.hpp"
```

Include dependency graph for fluid_simulation.hpp:



This graph shows which files directly or indirectly include this file:



Classes

- class [fluid_simulation](#)

5.1.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

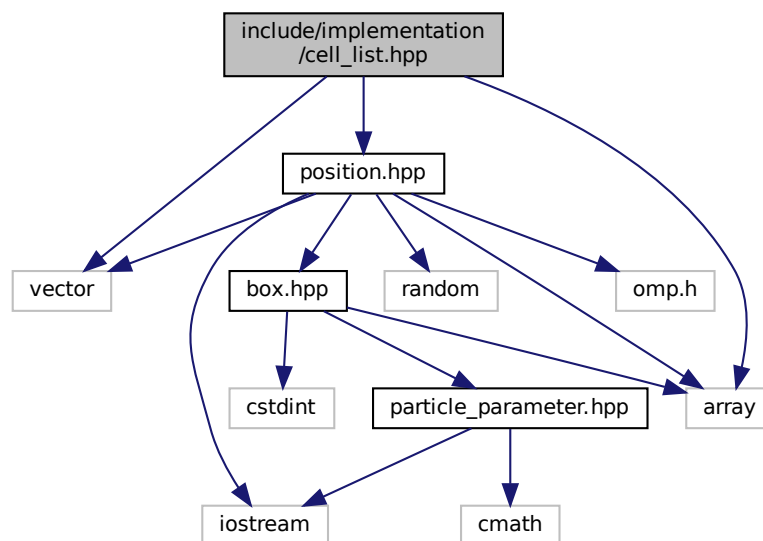
2021-12-26

Copyright

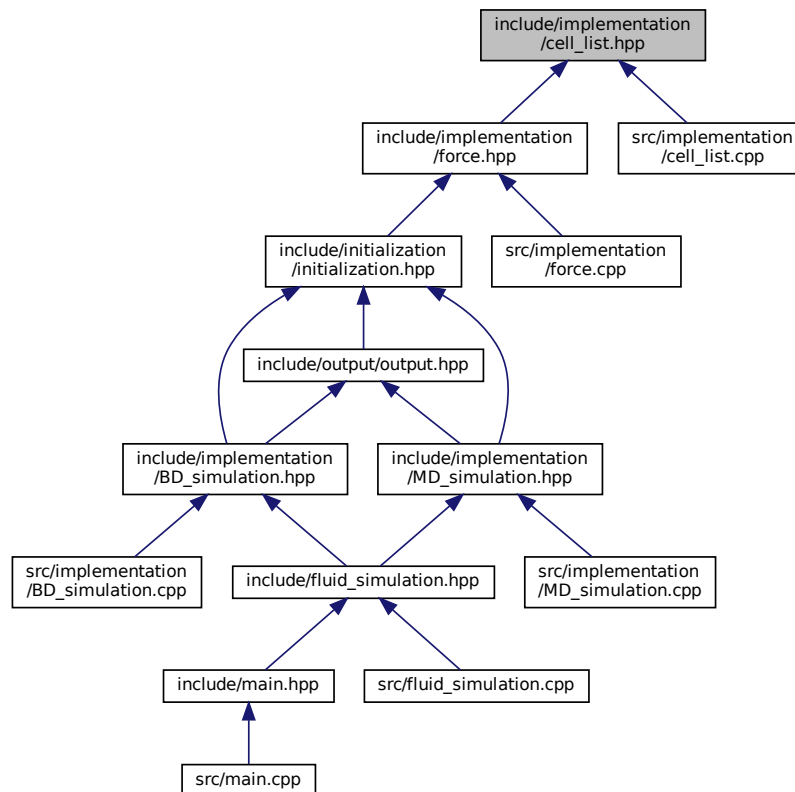
Copyright (c) 2021

5.2 include/implementation/cell_list.hpp File Reference

```
#include <array>
#include <vector>
#include "position.hpp"
Include dependency graph for cell_list.hpp:
```



This graph shows which files directly or indirectly include this file:



Classes

- class [cell_list](#)

5.2.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-26

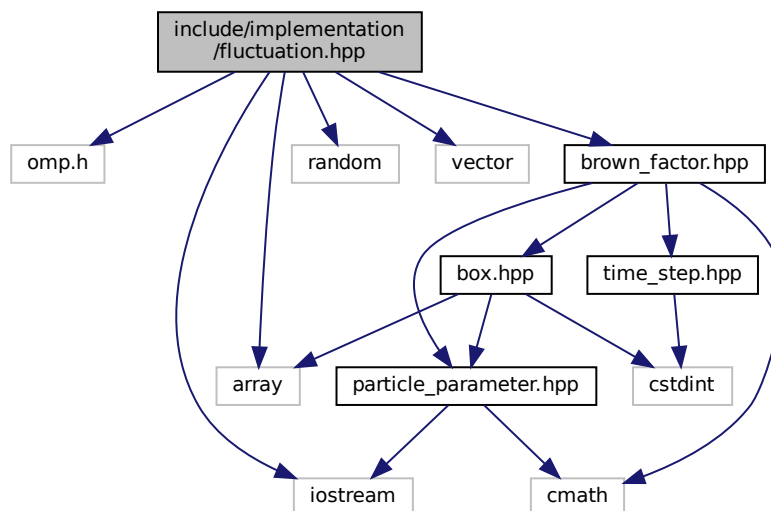
Copyright

Copyright (c) 2021

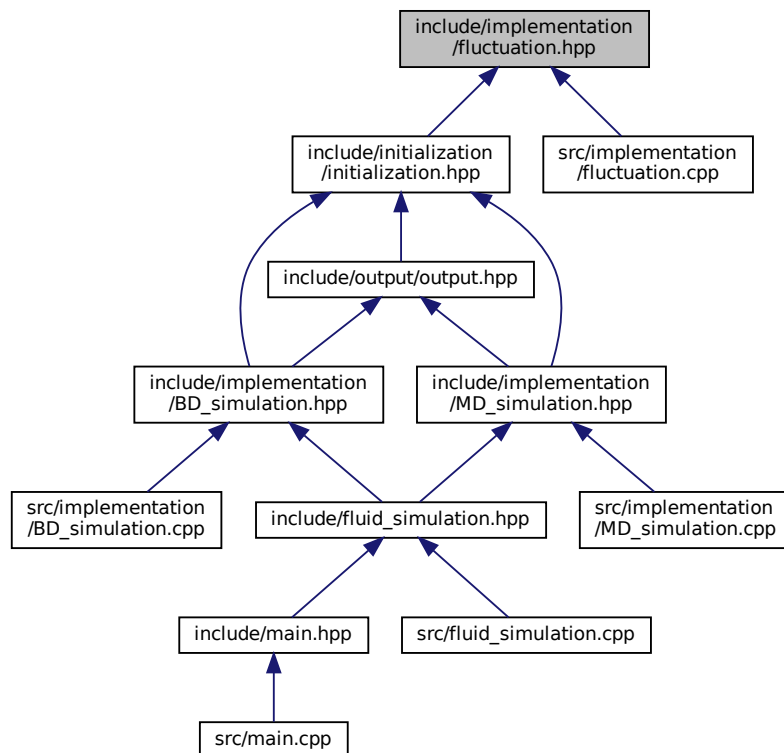
5.3 include/implementation/fluctuation.hpp File Reference

```
#include <omp.h>
#include <array>
#include <iostream>
#include <random>
#include <vector>
#include "brown_factor.hpp"
```

Include dependency graph for fluctuation.hpp:



This graph shows which files directly or indirectly include this file:



Classes

- class [fluctuation](#)

5.3.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

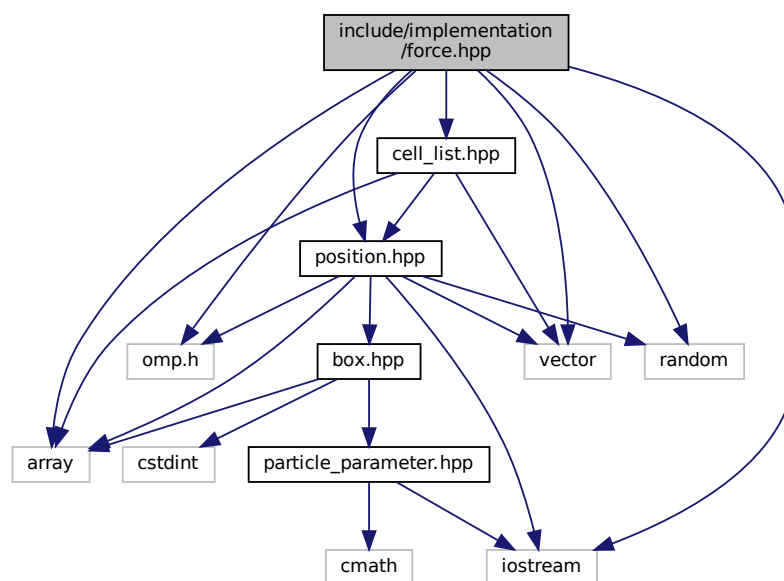
2021-12-23

Copyright

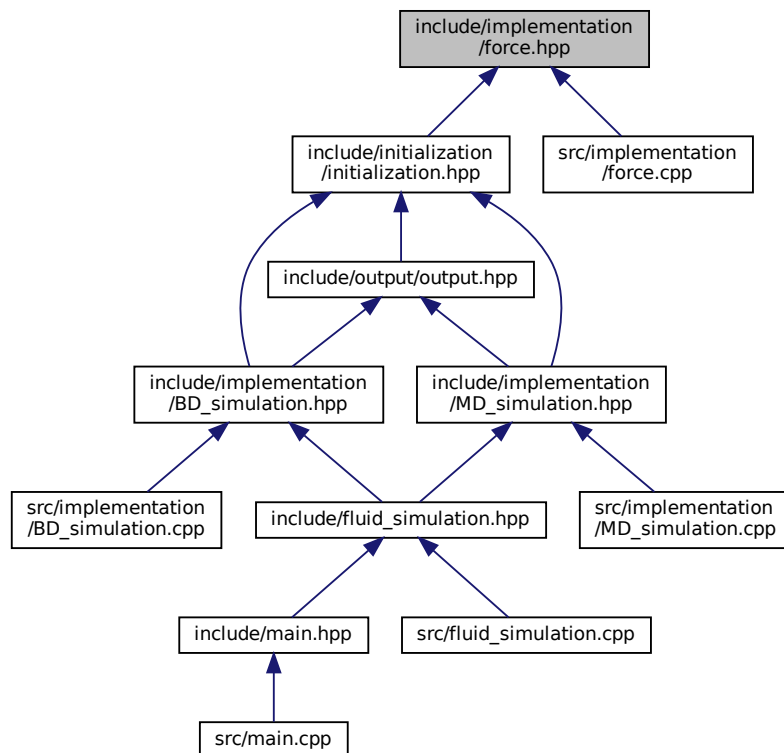
Copyright (c) 2021

5.4 include/implementation/force.hpp File Reference

```
#include <omp.h>
#include <array>
#include <iostream>
#include <random>
#include <vector>
#include "position.hpp"
#include "cell_list.hpp"
Include dependency graph for force.hpp:
```



This graph shows which files directly or indirectly include this file:



Classes

- class [force](#)

5.4.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

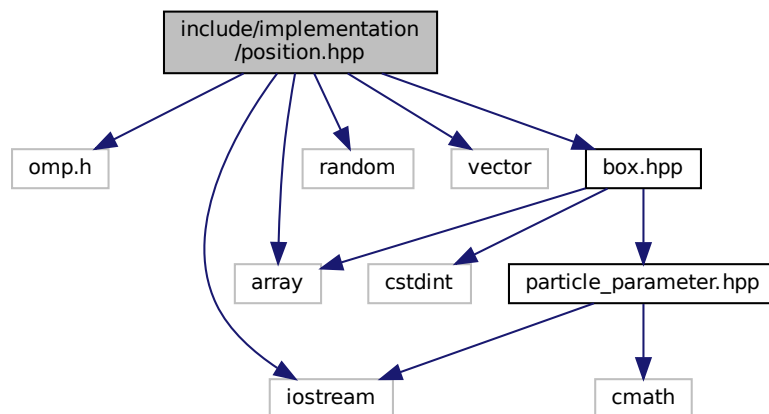
2021-12-23

Copyright

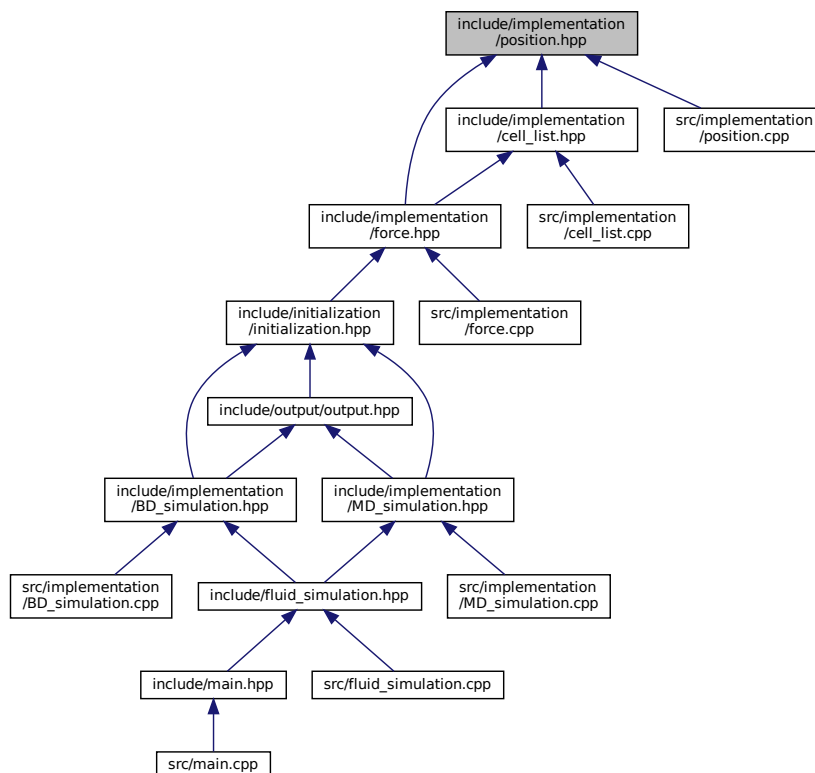
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5.5 include/implementation/position.hpp File Reference

```
#include <omp.h>
#include <array>
#include <iostream>
#include <random>
#include <vector>
#include "box.hpp"
Include dependency graph for position.hpp:
```



This graph shows which files directly or indirectly include this file:



Classes

- class [position](#)

5.5.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-23

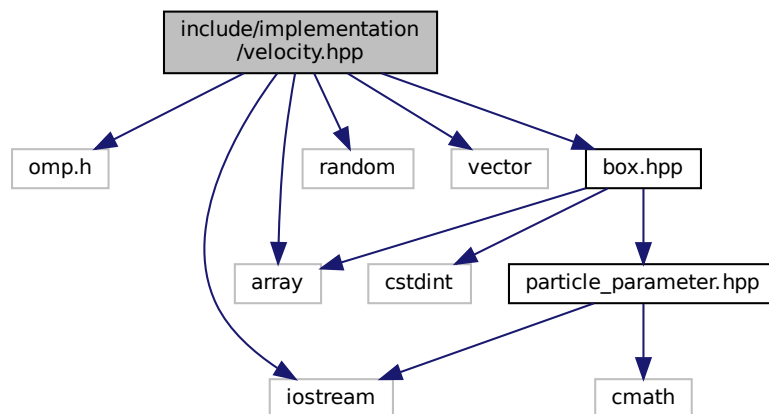
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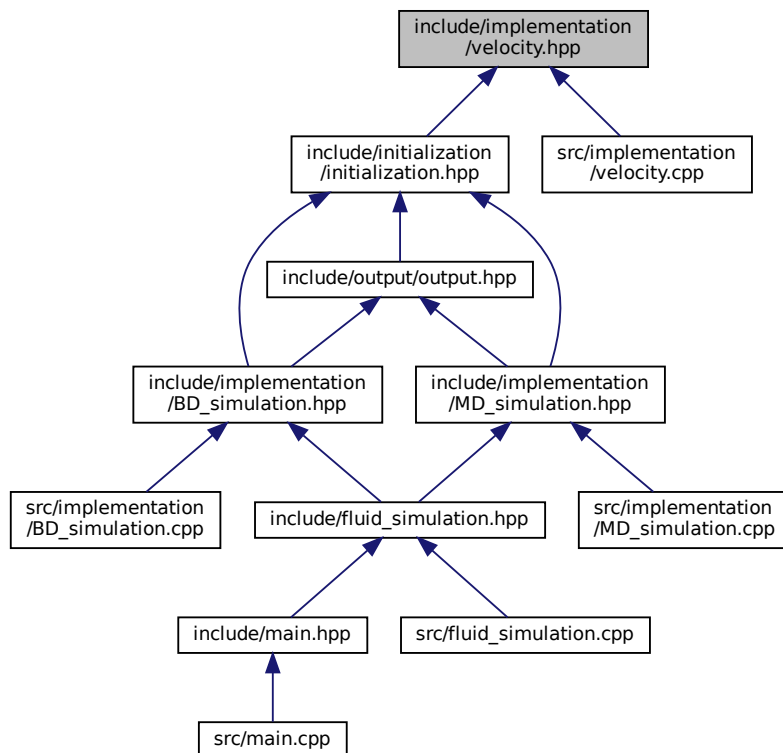
5.6 include/implementation/velocity.hpp File Reference

```
#include <omp.h>
#include <array>
#include <iostream>
#include <random>
#include <vector>
#include "box.hpp"
```

Include dependency graph for velocity.hpp:



This graph shows which files directly or indirectly include this file:



Classes

- class [velocity](#)

5.6.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

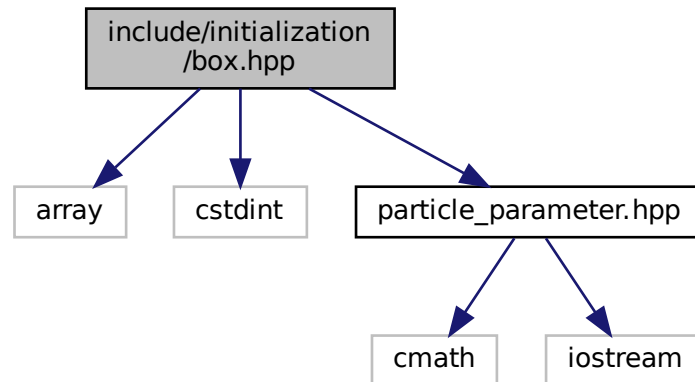
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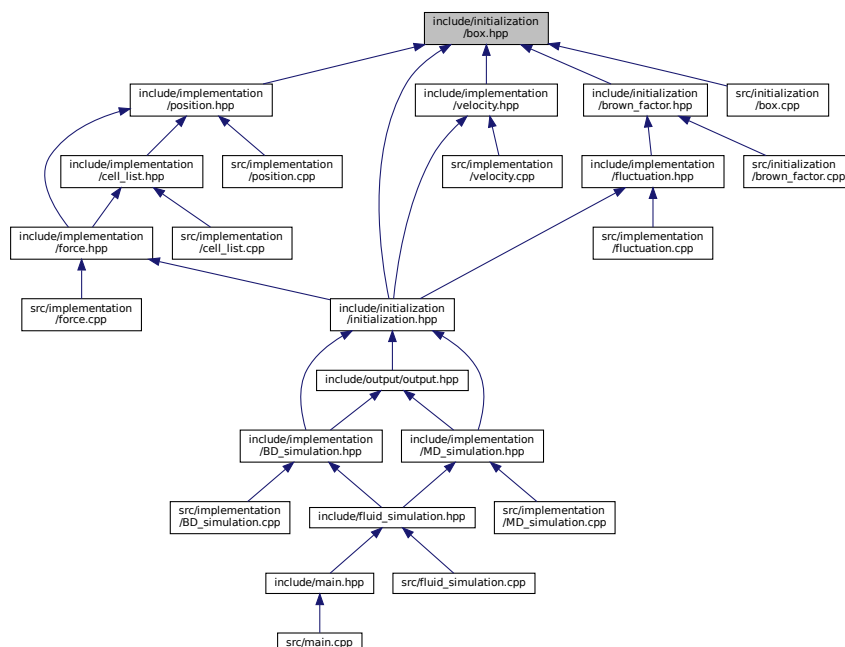
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5.7 include/initialization/box.hpp File Reference

```
#include <array>
#include <cstdint>
#include "particle_parameter.hpp"
Include dependency graph for box.hpp:
```



This graph shows which files directly or indirectly include this file:



Classes

- class [box](#)

5.7.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

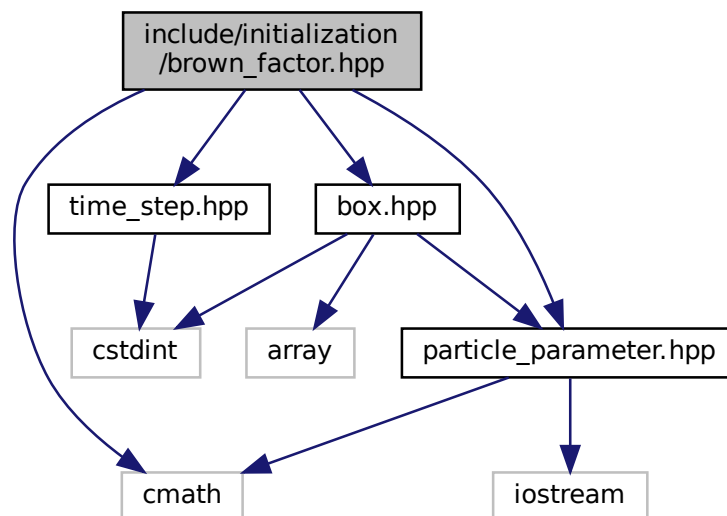
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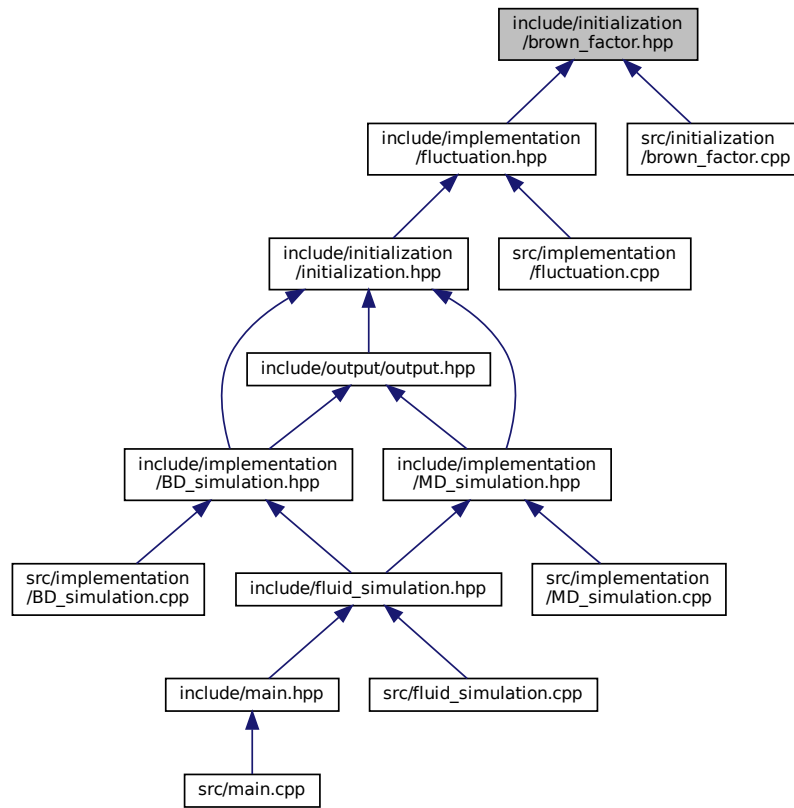
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5.8 include/initialization/brown_factor.hpp File Reference

```
#include <cmath>
#include "box.hpp"
#include "particle_parameter.hpp"
#include "time_step.hpp"
Include dependency graph for brown_factor.hpp:
```



This graph shows which files directly or indirectly include this file:



Classes

- class [brown_factor](#)

5.8.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-05

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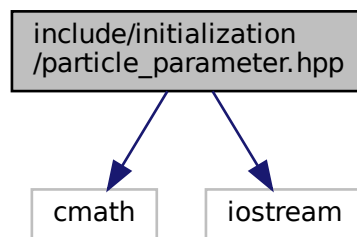
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5.9 include/initialization/particle_parameter.hpp File Reference

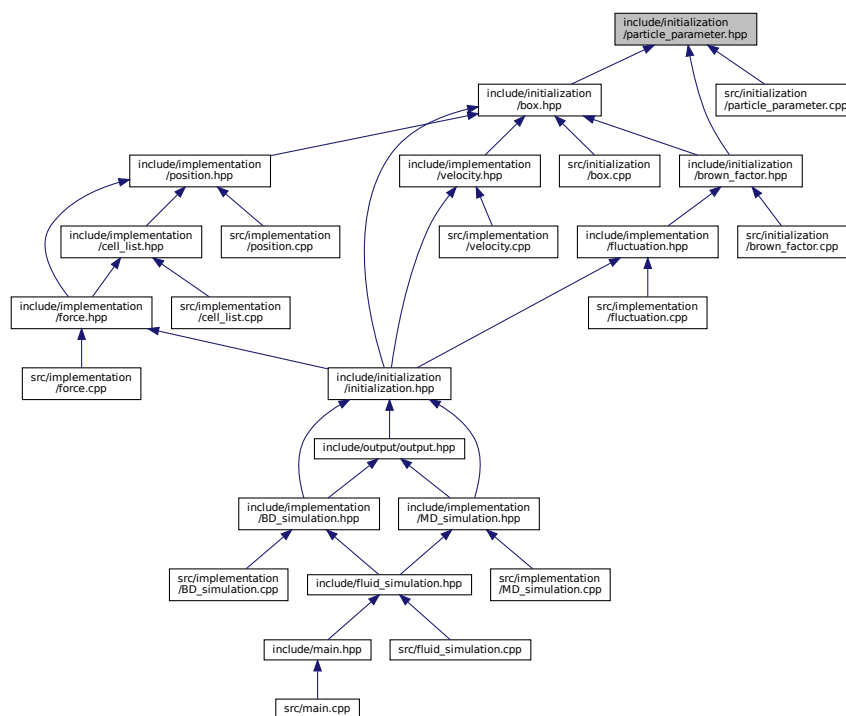
```
#include <cmath>
```

```
#include <iostream>
```

Include dependency graph for particle_parameter.hpp:



This graph shows which files directly or indirectly include this file:



Classes

- class [particle_parameter](#)

5.9.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-05

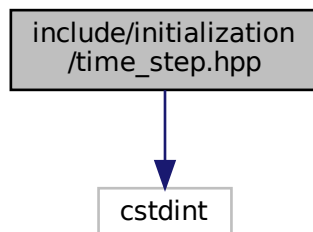
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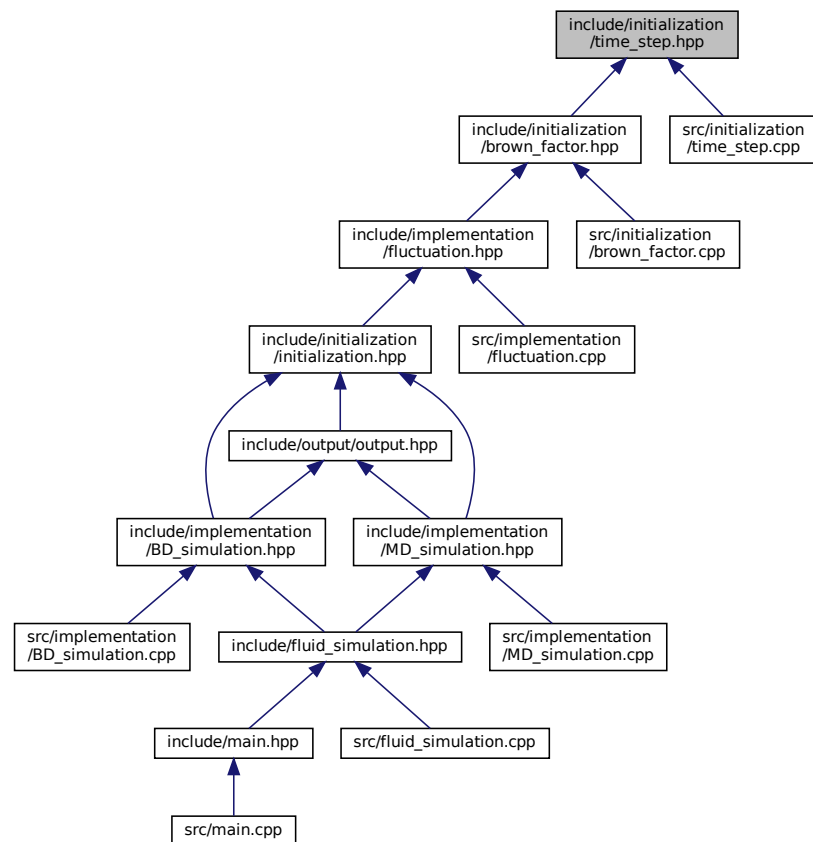
5.10 include/initialization/time_step.hpp File Reference

```
#include <cstdint>
```

Include dependency graph for time_step.hpp:



This graph shows which files directly or indirectly include this file:



Classes

- class [time_step](#)

5.10.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-05

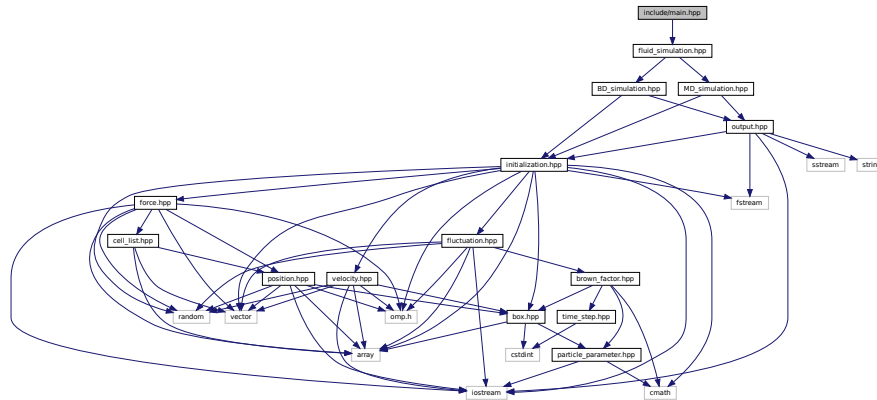
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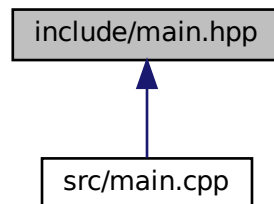
5.11 include/main.hpp File Reference

```
#include "fluid_simulation.hpp"
```

Include dependency graph for main.hpp:



This graph shows which files directly or indirectly include this file:



5.11.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

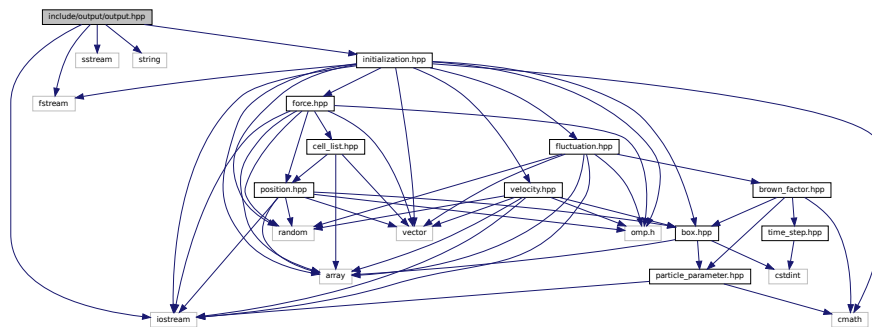
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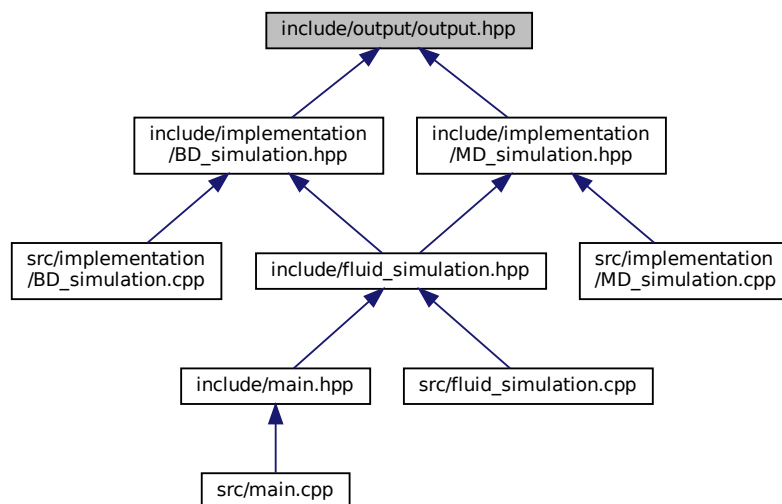
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5.12 include/output/output.hpp File Reference

```
#include <fstream>
#include <iostream>
#include <sstream>
#include <string>
#include "initialization.hpp"
Include dependency graph for output.hpp:
```



This graph shows which files directly or indirectly include this file:



Classes

- class [output](#)

5.12.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-26

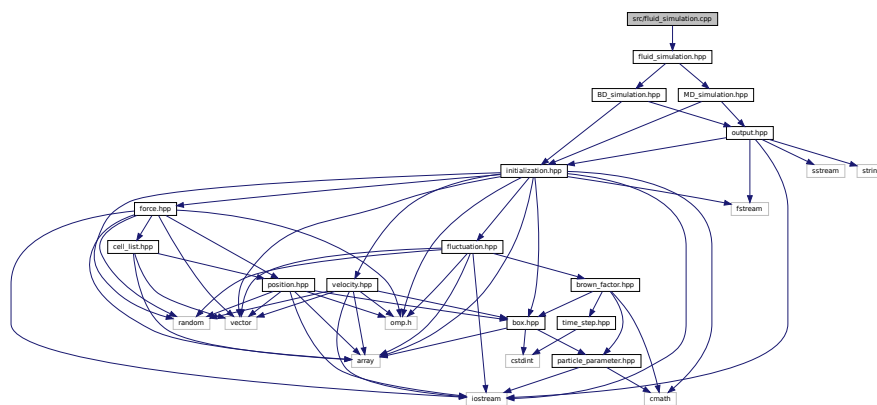
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5.13 src/fluid_simulation.cpp File Reference

```
#include "fluid_simulation.hpp"
```

Include dependency graph for fluid_simulation.cpp:



5.13.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-26

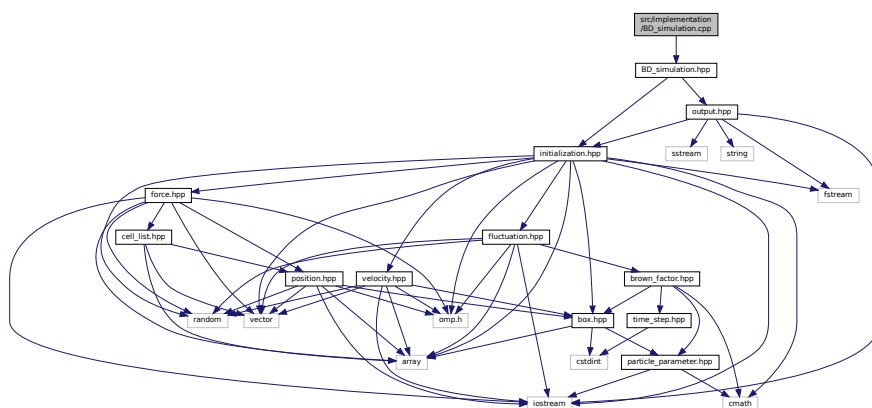
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5.14 src/implementation/BD_simulation.cpp File Reference

```
#include "BD_simulation.hpp"
```

Include dependency graph for BD_simulation.cpp:



5.14.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-26

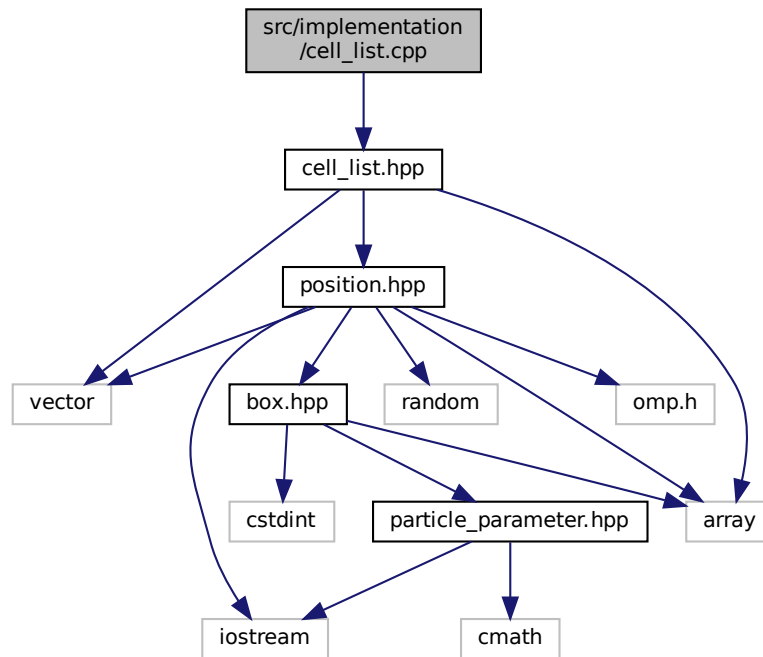
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5.15 src/implementation/cell_list.cpp File Reference

```
#include "cell_list.hpp"
```

Include dependency graph for cell_list.cpp:



5.15.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

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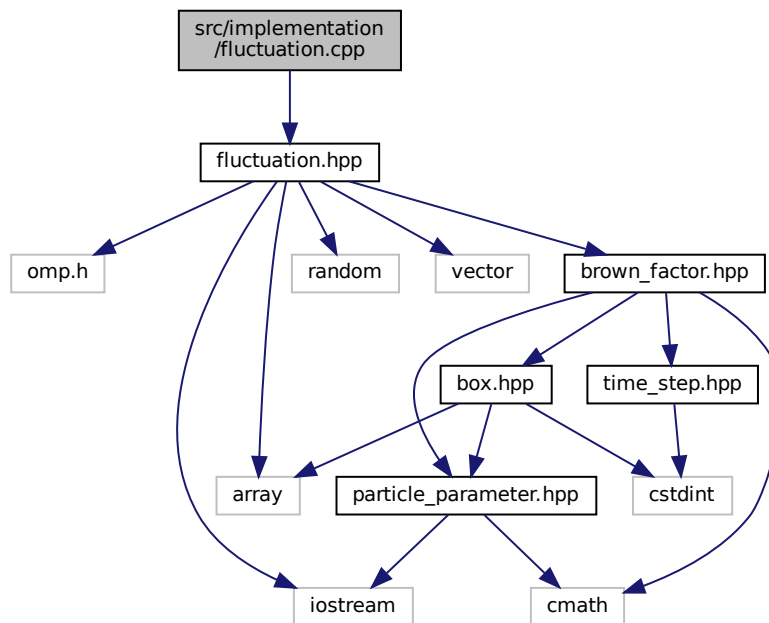
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5.16 src/implementation/fluctuation.cpp File Reference

```
#include "fluctuation.hpp"
```

Include dependency graph for fluctuation.cpp:



5.16.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

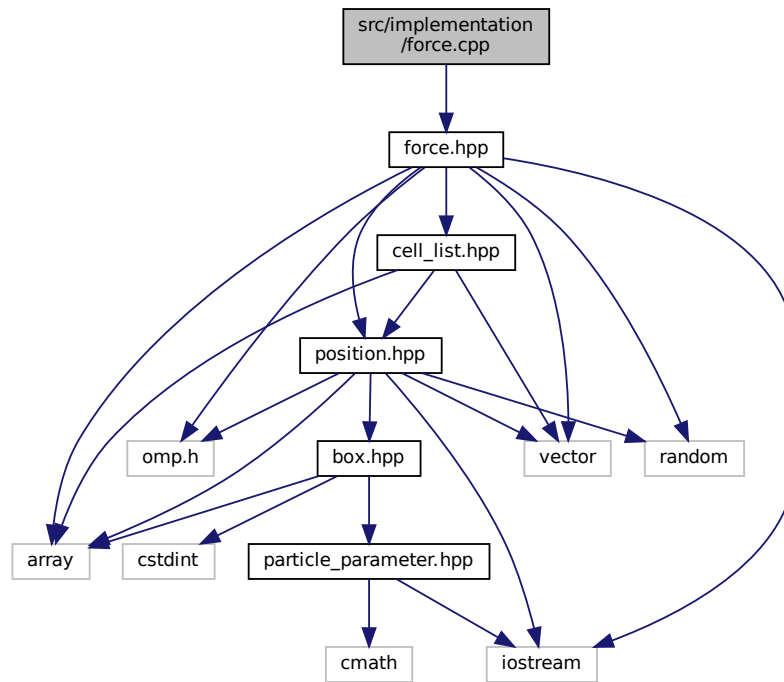
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Copyright

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5.17 src/implementation/force.cpp File Reference

```
#include "force.hpp"  
Include dependency graph for force.cpp:
```



5.17.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-23

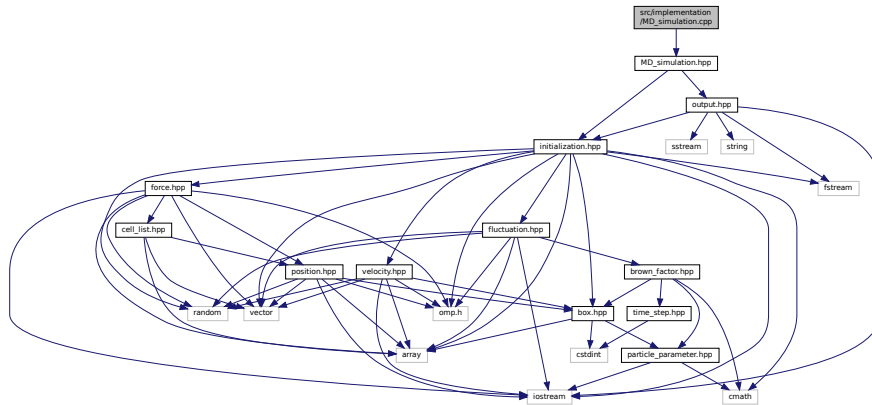
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5.18 src/implementation/MD_simulation.cpp File Reference

```
#include "MD_simulation.hpp"
```

Include dependency graph for MD_simulation.cpp:



5.18.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-26

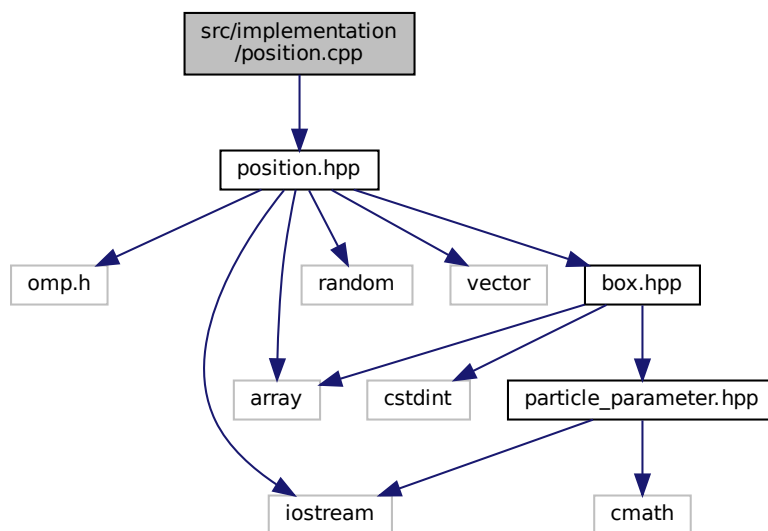
Copyright

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5.19 src/implementation/position.cpp File Reference

```
#include "position.hpp"
```

Include dependency graph for position.cpp:



5.19.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-23

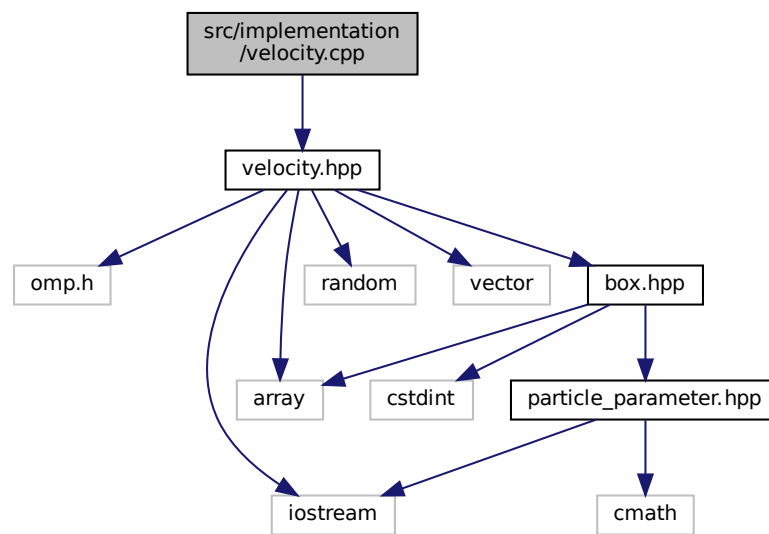
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5.20 src/implementation/velocity.cpp File Reference

```
#include "velocity.hpp"
```

Include dependency graph for velocity.cpp:



5.20.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-23

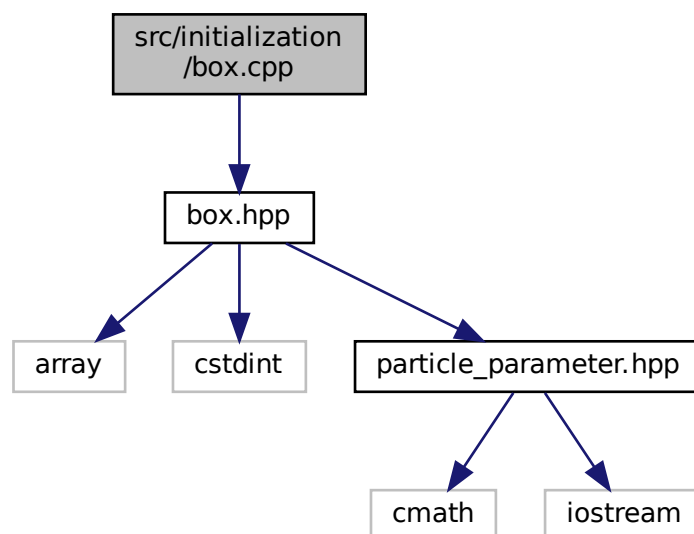
Copyright

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5.21 src/initialization/box.cpp File Reference

```
#include "box.hpp"
```

Include dependency graph for box.cpp:



5.21.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-06

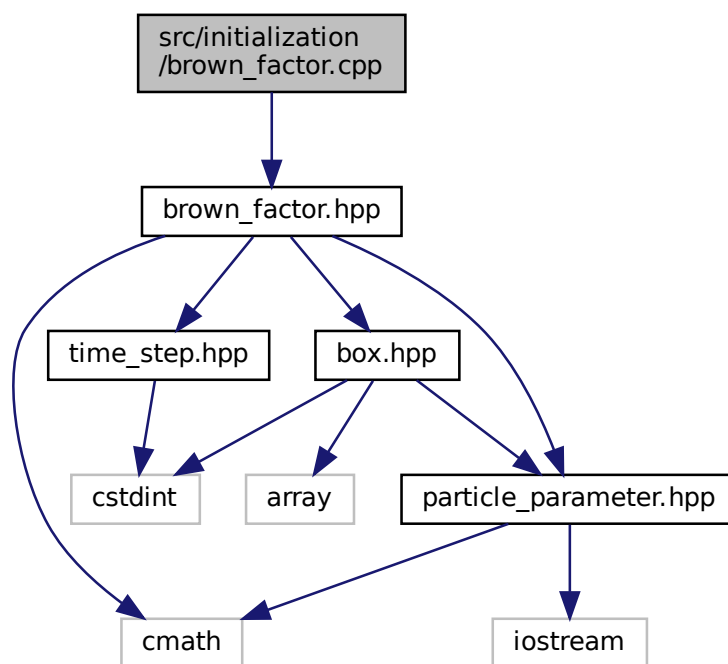
Copyright

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5.22 src/initialization/brown_factor.cpp File Reference

```
#include "brown_factor.hpp"
```

Include dependency graph for brown_factor.cpp:



5.22.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

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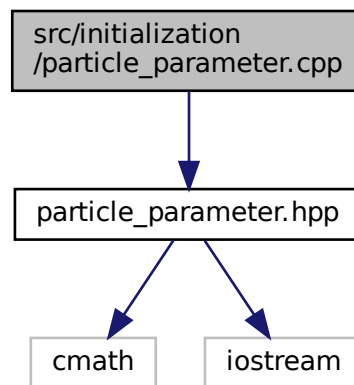
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5.23 src/initialization/particle_parameter.cpp File Reference

```
#include "particle_parameter.hpp"
```

Include dependency graph for particle_parameter.cpp:



5.23.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

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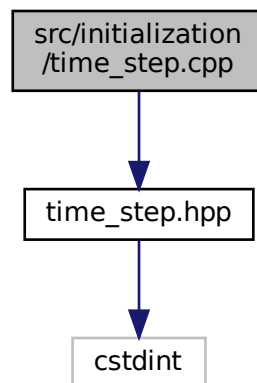
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5.24 src/initialization/time_step.cpp File Reference

```
#include "time_step.hpp"
```

Include dependency graph for time_step.cpp:



5.24.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-12-05

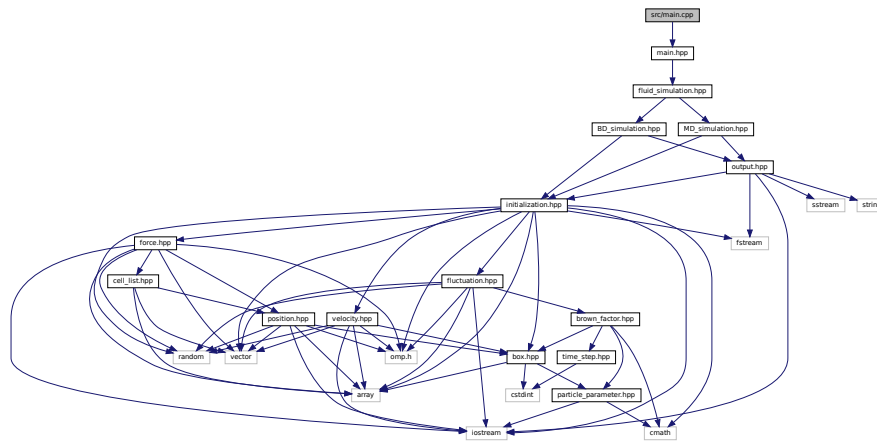
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5.25 src/main.cpp File Reference

```
#include "main.hpp"
```

Include dependency graph for main.cpp:



Functions

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

5.25.1 Detailed Description

Author

Haoran Chen (chen950302@live.com)

Version

0.1

Date

2021-09-16

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