Gross-Pitaevskii-FDM

0.1

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Chapter 1

Hierarchical Index

1.1 Class Hierarchy

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

Chapter 2

Class Index

2.1 Class List

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

Chapter 3

File Index

3.1 File List

Here is a list of all files with brief descriptions:

Chapter 4

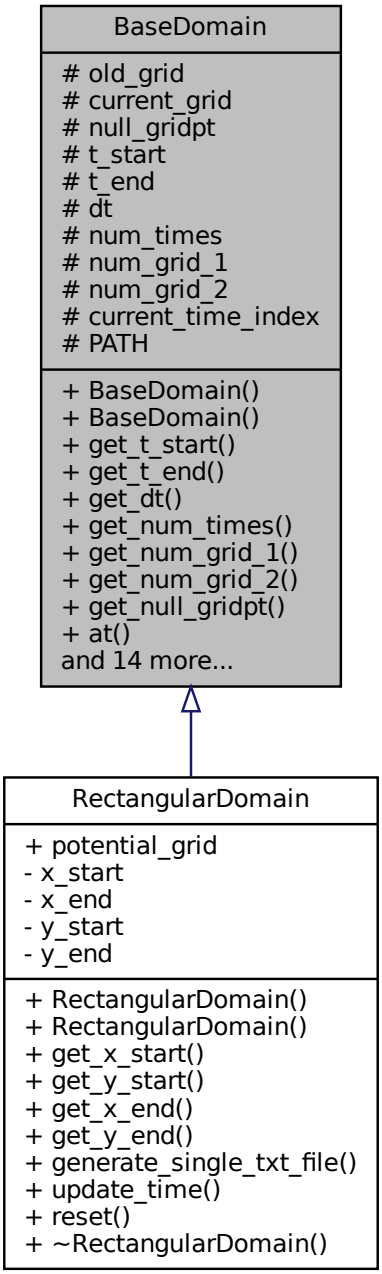
Class Documentation

4.1 BaseDomain Class Reference

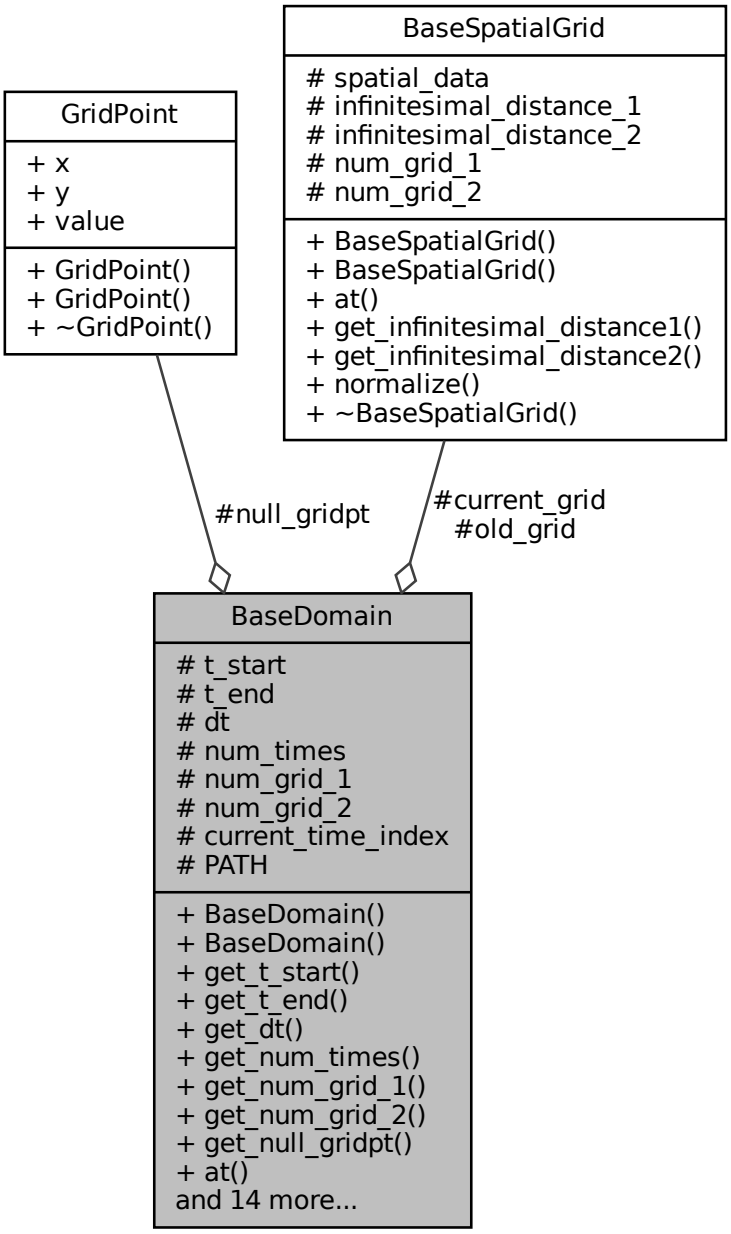
Base domain class containing multiple time steps and export methods.

```
#include <base_domain.h>
```

Inheritance diagram for BaseDomain:



Collaboration diagram for BaseDomain:



Public Member Functions

- BaseDomain ()
- BaseDomain (int num_grid_1, int num_grid_2, float t_start, float t_end, int num_times)
- float get_t_start ()
- float get_t_end ()
- float get_dt ()
- int get_num_times ()

- int get_num_grid_1 ()
- int get_num_grid_2 ()
- GridPoint * get_null_gridpt ()
- GridPoint * at (int index_1, int index_2, int time_index)
- void assign_initial_value (int index_1, int index_2, std::complex< float > value)

  Assign initial value.
- void assign_wave_function (int index_1, int index_2, int time_index, std::complex< float > value)
- float time_at (int time_index)
- float get_infinitesimal_distance1 ()
- float get_infinitesimal_distance2 ()
- void generate_directory_name (std::string info, bool print_info=true)

  create directory and return directory name with "/" directory name : "./results/%d-%m-%Y %H-%M-%S_"+info for exmaple, "./results/"
- void generate_single_txt_file (std::string filename, bool cuda_mode=false)

  export results of probability(|psi|^2) as txt it generates (num_times) txt files each txt file contains |psi|^2 data
- void normalize (int time_index)
- void print_directory_info ()
- int get_current_time_index ()
- ~BaseDomain ()
- std::string get_path ()
- void update_time (bool cuda_mode=false)
- virtual void reset ()

Protected Attributes

- BaseSpatialGrid * old_grid
- BaseSpatialGrid * current_grid
- GridPoint * null_gridpt
- float t_start
- float t_end
- float dt
- int num_times
- int num_grid_1
- int num_grid_2
- int current_time_index = 0
- std::string PATH

4.1.1 Detailed Description

Base domain class containing multiple time steps and export methods.

Definition at line 67 of file base_domain.h.

4.1.2 Constructor & Destructor Documentation

4.1.2.1 BaseDomain() [1/2]

```
BaseDomain::BaseDomain ( )
```

4.1.2.2 BaseDomain() [2/2]

```
BaseDomain::BaseDomain (
            int num_grid_1,
            int num_grid_2,
            float t_start,
            float t_end,
            int num_times )
```

Definition at line 81 of file base_domain.cpp.

```
87 {
88     this->t_start = t_start;
89     this->t_end = t_end;
90     this->num_times = num_times;
91     // dt: interval of time
92     this->dt = (t_end - t_start) / (num_times - 1);
93     this->num_grid_1 = num_grid_1;
94     this->num_grid_2 = num_grid_2;
95     this->old_grid = new BaseSpatialGrid(num_grid_1, num_grid_2);
96     this->current_grid = new BaseSpatialGrid(num_grid_1, num_grid_2);
97     this->null_gridpt = new GridPoint(0, 0, std::complex<float>{0});
98 }
```

4.1.2.3 ~BaseDomain()

```
BaseDomain::~BaseDomain ( )
```

Definition at line 100 of file base_domain.cpp.

```
101 {
102     delete (this->old_grid);
103     delete (this->current_grid);
104 }
```

4.1.3 Member Function Documentation

4.1.3.1 assign_initial_value()

```
void BaseDomain::assign_initial_value (
            int index_1,
            int index_2,
            std::complex< float > value )
```

Assign initial value.

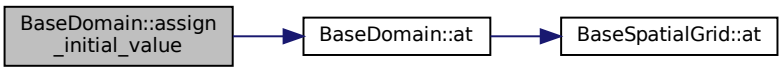
Parameters

index_1	x = x_start + index_1∗dx
index_2	y = y_start + index_2 ∗ dy
value	initial value at x, y

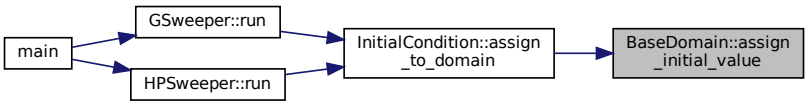
Definition at line 188 of file base_domain.cpp.

```
189 {
190     this->at(index_1, index_2, 0)->value = value;
191 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



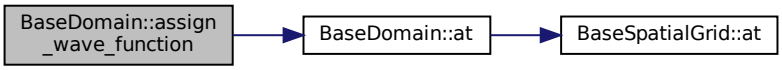
4.1.3.2 assign_wave_function()

```
void BaseDomain::assign_wave_function (
            int index_1,
            int index_2,
            int time_index,
            std::complex< float > value )
```

Definition at line 192 of file base_domain.cpp.

```
193 {
194     this->at(index_1, index_2, time_index)->value = value;
195 }
```

Here is the call graph for this function:



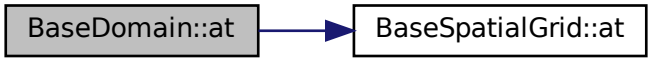
4.1.3.3 at()

```
GridPoint * BaseDomain::at (
            int index_1,
            int index_2,
            int time_index )
```

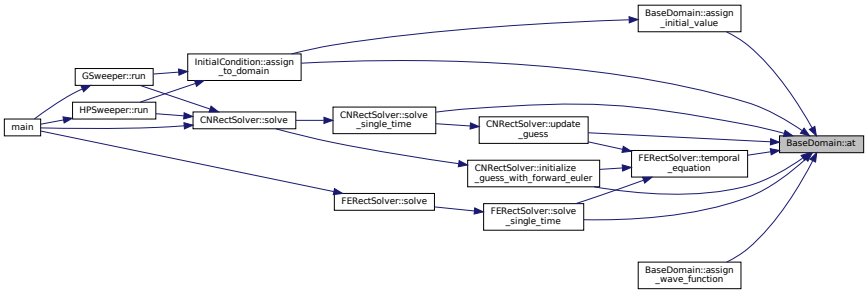
Definition at line 153 of file base_domain.cpp.

```
154 {
155     if (time_index == this->current_time_index)
156     {
157         return this->current_grid->at(index_1, index_2);
158     }
159     else if (time_index == this->current_time_index - 1)
160     {
161         return this->old_grid->at(index_1, index_2);
162     }
163     else
164     {
165         std::cerr << "error in base domin at function" << std::endl;
166         return this->current_grid->at(index_1, index_2);
167     }
168 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.1.3.4 generate_directory_name()

```
void BaseDomain::generate_directory_name (
            std::string info,
            bool print_info = true )
```

create directory and return directory name with "/" directory name : "./results/%d-%m-%Y %H-%M-%S_"+info for exmaple, "./results/"

Parameters

info	information about domain type and solver type

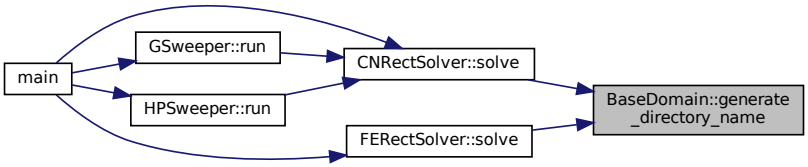
Returns

std::string directory name with "/"

Definition at line 203 of file base_domain.cpp.

```
204 {
205     auto t = std::time(nullptr);
206     auto tm = *std::localtime(&t);
207 
208     std::ostringstream oss;
209     oss << std::put_time(&tm, "%Y-%m-%d-%H-%M-%S");
210     auto str = oss.str();
211     std::string directory_name = "../results/" + str + "_" + info;
212     bool created = fs::create_directory(directory_name.c_str());
213     if (print_info && created)
214     {
215         std::cout << "Created directory " << directory_name << std::endl;
216     }
217     // else if(print_info )
218     //TODO
219     else if (!created)
220     {
221         std::cout << "Creating directory failed" << std::endl;
222     }
223 
224     this->PATH = directory_name + "/";
225 }
```

Here is the caller graph for this function:



4.1.3.5 generate_single_txt_file()

```
void BaseDomain::generate_single_txt_file (
            std::string filename,
            bool cuda_mode = false )
```

export results of probability(|psi|^2) as txt it generates (num_times) txt files each txt file contains |psi|^2 data

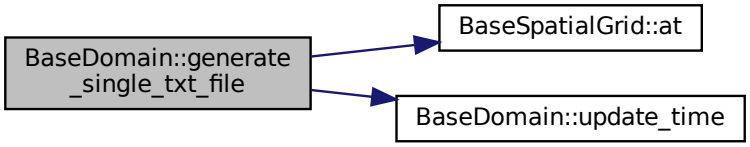
Parameters

grid	grid at t
filename	file name to store data

Definition at line 235 of file base_domain.cpp.

```
236 {
237     if (cuda_mode){
238         this->update_time(cuda_mode);
239     }
240     else{
241         std::ofstream outfile(this->PATH + filename + ".txt");
242         outfile « "x, y, real, imag, magn, phase " « std::endl;
243         for (auto i = 0; i < num_grid_1; ++i)
244         {
245             for (auto j = 0; j < num_grid_2; ++j)
246             {
247                 float magnitude = std::abs(this->current_grid->at(i, j)->value);
248                 float phase = std::arg(this->current_grid->at(i, j)->value);
249                 outfile « this->current_grid->at(i, j)->x « ", " « this->current_grid->at(i, j)->y « ",
    ";
250                 outfile « this->current_grid->at(i, j)->value.real() « ", " « this->current_grid->at(i,
    j)->value.imag() « ", ";
251                 outfile « magnitude « ", " « phase;
252                 outfile « std::endl;
253             }
254         }
255         outfile.close();
256         // After saving data, update domain
257         this->update_time();
258     }
259 };
```

Here is the call graph for this function:



4.1.3.6 get_current_time_index()

```
int BaseDomain::get_current_time_index ( )
```

Definition at line 170 of file base_domain.cpp.

```
171 {
172     return this->current_time_index;
173 }
```

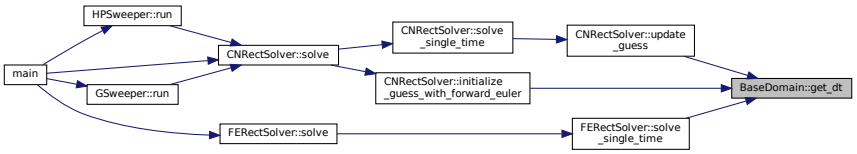
4.1.3.7 get_dt()

```
float BaseDomain::get_dt ( )
```

Definition at line 125 of file base_domain.cpp.

```
126 {
127     return this->dt;
128 }
```

Here is the caller graph for this function:



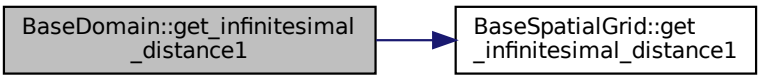
4.1.3.8 get_infinitesimal_distance1()

```
float BaseDomain::get_infinitesimal_distance1 ( )
```

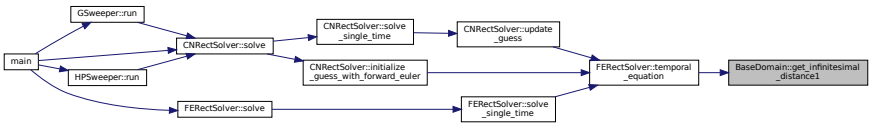
Definition at line 143 of file base_domain.cpp.

```
144 {
145     return this->old_grid->get_infinitesimal_distance1();
146 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



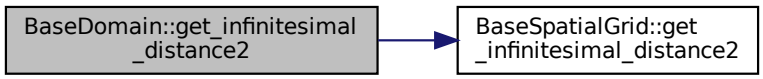
4.1.3.9 get_infinitesimal_distance2()

```
float BaseDomain::get_infinitesimal_distance2 ( )
```

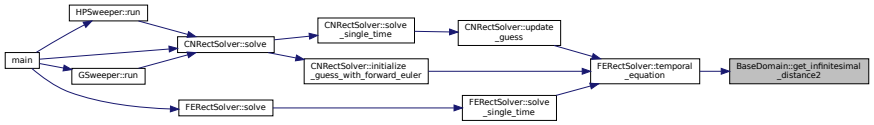
Definition at line 147 of file base_domain.cpp.

```
148 {
149     return this->old_grid->get_infinitesimal_distance2();
150 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



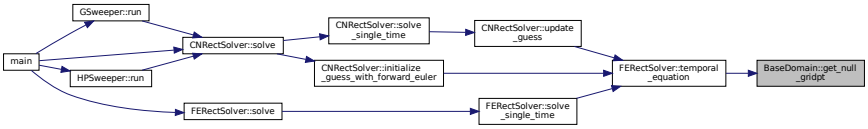
4.1.3.10 get_null_gridpt()

```
GridPoint * BaseDomain::get_null_gridpt ( )
```

Definition at line 176 of file base_domain.cpp.

```
177 {
178     return this->null_gridpt;
179 }
```

Here is the caller graph for this function:



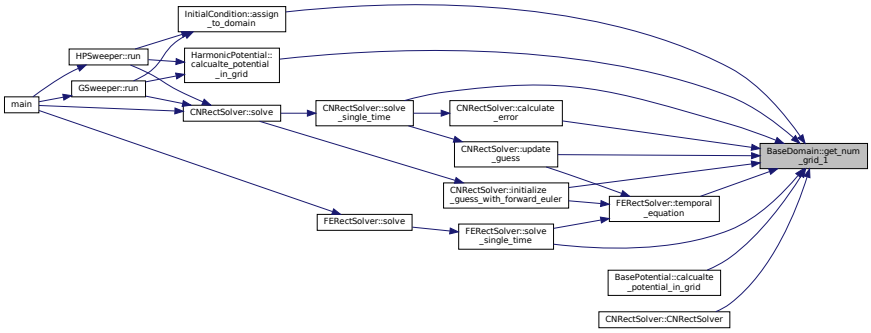
4.1.3.11 get_num_grid_1()

```
int BaseDomain::get_num_grid_1 ( )
```

Definition at line 134 of file base_domain.cpp.

```
135 {
136     return this->num_grid_1;
137 }
```

Here is the caller graph for this function:



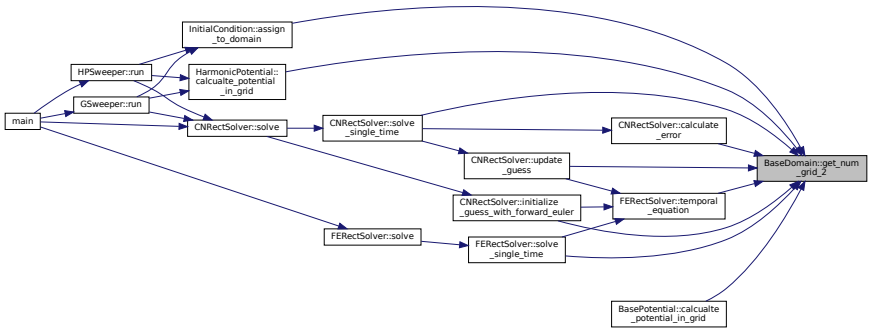
4.1.3.12 get_num_grid_2()

```
int BaseDomain::get_num_grid_2 ( )
```

Definition at line 138 of file base_domain.cpp.

```
139 {
140     return this->num_grid_2;
141 }
```

Here is the caller graph for this function:



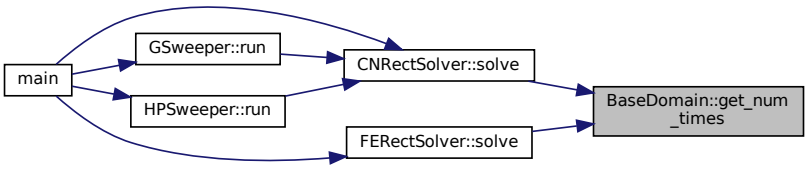
4.1.3.13 get_num_times()

```
int BaseDomain::get_num_times ( )
```

Definition at line 129 of file base_domain.cpp.

```
130 {
131     return this->num_times;
132 }
```

Here is the caller graph for this function:



4.1.3.14 get_path()

```
std::string BaseDomain::get_path ( )
```

Definition at line 106 of file base_domain.cpp.

```
107 {
108     return this->PATH;
109 }
```

4.1.3.15 get_t_end()

```
float BaseDomain::get_t_end ( )
```

Definition at line 121 of file base_domain.cpp.

```
122 {
123     return this->t_end;
124 }
```

4.1.3.16 get_t_start()

```
float BaseDomain::get_t_start ( )
```

Definition at line 116 of file base_domain.cpp.

```
117 {
118     return this->t_start;
119 }
```

4.1.3.17 normalize()

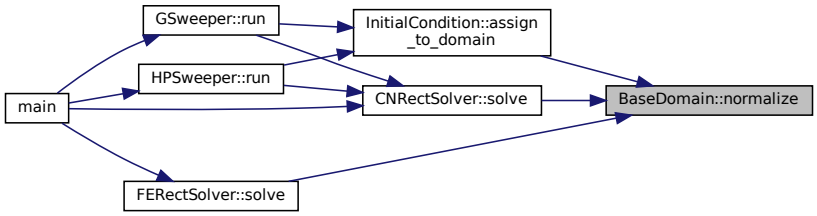
```
void BaseDomain::normalize (
            int time_index )
```

Definition at line 111 of file base_domain.cpp.

```
112 {
113     this->current_grid->normalize();
114 }
```

Here is the call graph for this function:

Here is the caller graph for this function:



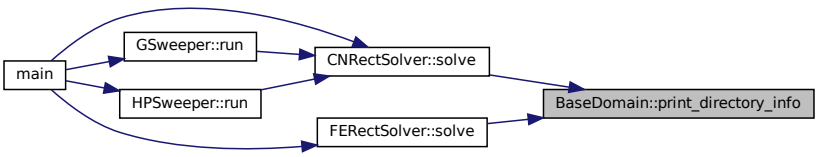
4.1.3.18 print_directory_info()

```
void BaseDomain::print_directory_info ( )
```

Definition at line 261 of file base_domain.cpp.

```
262 {
263     std::cout « this->num_times;
264     std::cout « " text files are generated in \n";
265     std::cout « this->PATH « std::endl;
266 }
```

Here is the caller graph for this function:



4.1.3.19 reset()

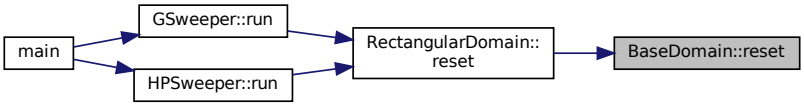
```
void BaseDomain::reset ( )  [virtual]
```

Reimplemented in RectangularDomain.

Definition at line 282 of file base_domain.cpp.

```
283 {
284     this->current_time_index = 0;
285     delete this->old_grid;
286     delete this->current_grid;
287 
288     this->current_grid = new BaseSpatialGrid(num_grid_1, num_grid_2);
289     this->old_grid = new BaseSpatialGrid(num_grid_1, num_grid_2);
290 }
```

Here is the caller graph for this function:



4.1.3.20 time_at()

```
float BaseDomain::time_at (
            int time_index )
```

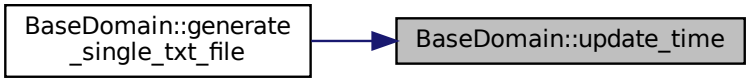
4.1.3.21 update_time()

```
void BaseDomain::update_time (
            bool cuda_mode = false )
```

Definition at line 268 of file base_domain.cpp.

```
269 {
270     if (cuda_mode){
271         this->current_time_index += 1;
272     }
273     else{
274 
275         this->current_time_index += 1;
276         delete (this->old_grid);
277         this->old_grid = this->current_grid;
278         this->current_grid = new BaseSpatialGrid(num_grid_1, num_grid_2);
279     }
280 }
```

Here is the caller graph for this function:



4.1.4 Member Data Documentation

4.1.4.1 current_grid

```
BaseSpatialGrid* BaseDomain::current_grid  [protected]
```

Definition at line 98 of file base_domain.h.

4.1.4.2 current_time_index

```
int BaseDomain::current_time_index = 0  [protected]
```

Definition at line 102 of file base_domain.h.

4.1.4.3 dt

```
float BaseDomain::dt  [protected]
```

Definition at line 100 of file base_domain.h.

4.1.4.4 null_gridpt

```
GridPoint* BaseDomain::null_gridpt  [protected]
```

Definition at line 99 of file base_domain.h.

4.1.4.5 num_grid_1

```
int BaseDomain::num_grid_1  [protected]
```

Definition at line 101 of file base_domain.h.

4.1.4.6 num_grid_2

```
int BaseDomain::num_grid_2  [protected]
```

Definition at line 101 of file base_domain.h.

4.1.4.7 num_times

```
int BaseDomain::num_times  [protected]
```

Definition at line 101 of file base_domain.h.

4.1.4.8 old_grid

```
BaseSpatialGrid* BaseDomain::old_grid  [protected]
```

Definition at line 97 of file base_domain.h.

4.1.4.9 PATH

```
std::string BaseDomain::PATH  [protected]
```

Definition at line 103 of file base_domain.h.

4.1.4.10 t_end

```
float BaseDomain::t_end  [protected]
```

Definition at line 100 of file base_domain.h.

4.1.4.11 t_start

```
float BaseDomain::t_start  [protected]
```

Definition at line 100 of file base_domain.h.

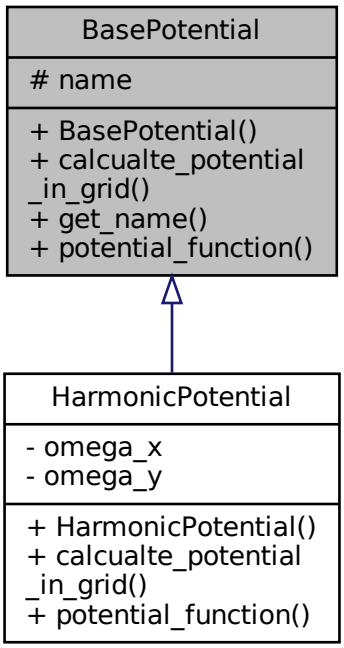
The documentation for this class was generated from the following files:

- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/domain/base_domain.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/domain/base_domain.cpp

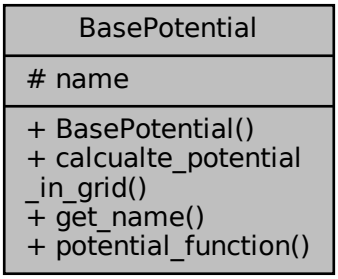
4.2 BasePotential Class Reference

`#include <base_potential.h>`

Inheritance diagram for BasePotential:



Collaboration diagram for BasePotential:



Public Member Functions

- BasePotential ()=default
- void calcualte_potential_in_grid (RectangularDomain *domain)

  Calculate potential values in each grid based on domain point coordinate and potential function.
- std::string get_name ()

  Getter for name class variable.
- float potential_function (float, float)

  Default potental function for constant zero potential.

Protected Attributes

- std::string name

4.2.1 Detailed Description

Definition at line 18 of file base_potential.h.

4.2.2 Constructor & Destructor Documentation

4.2.2.1 BasePotential()

```
BasePotential::BasePotential ( )  [default]
```

4.2.3 Member Function Documentation

4.2.3.1 calcualte_potential_in_grid()

```
void BasePotential::calcualte_potential_in_grid (
            RectangularDomain * domain )
```

Calculate potential values in each grid based on domain point coordinate and potential function.

Parameters

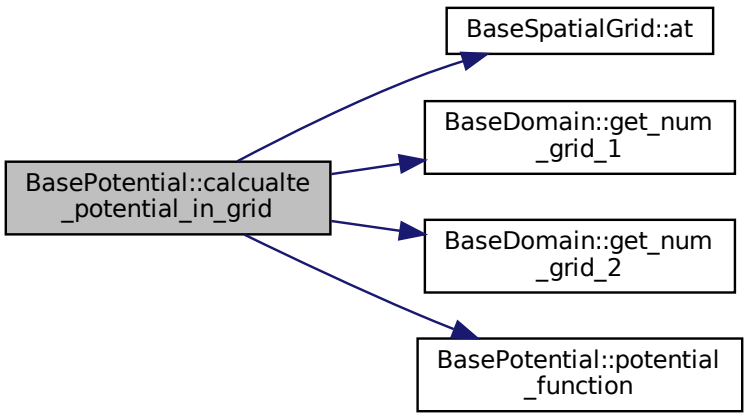
domain	

Definition at line 18 of file base_potential.cpp.

```
19 {
20     int num_grid_1 = domain->get_num_grid_1();
21     int num_grid_2 = domain->get_num_grid_2();
```

```
22     for (auto i = 0; i < num_grid_1; ++i)
23     {
24         for (auto j = 0; j < num_grid_2; ++j)
25         {
26             auto point = domain->potential_grid->at(i, j);
27 
28             //Assign potential value in potential grid
29             point->value = std::complex<float>{this->potential_function(point->x, point->y), 0};
30         }
31     }
32 
33 }
```

Here is the call graph for this function:



4.2.3.2 get_name()

```
std::string BasePotential::get_name ( )
```

Getter for name class variable.

Returns

std::string

Definition at line 40 of file base_potential.cpp.

```
41 {
42     return this->name;
43 }
```

4.2.3.3 potential_function()

```
float BasePotential::potential_function (
            float x,
            float y )
```

Default potental function for constant zero potential.

Parameters

x	
y	

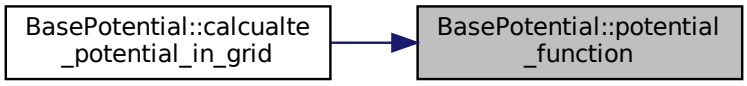
Returns

float

Definition at line 52 of file base_potential.cpp.

```
53 {
54     return 0;
55 }
```

Here is the caller graph for this function:



4.2.4 Member Data Documentation

4.2.4.1 name

```
std::string BasePotential::name  [protected]
```

Definition at line 27 of file base_potential.h.

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

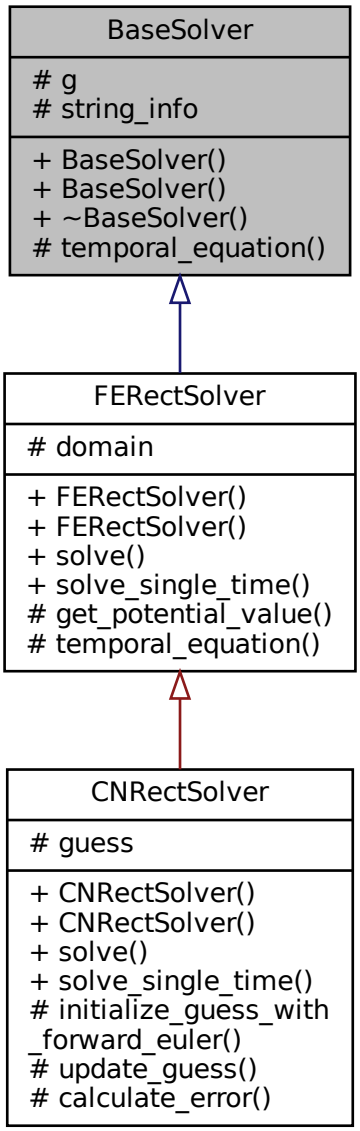
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/potential/base_potential.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/potential/base_potential.cpp

4.3 BaseSolver Class Reference

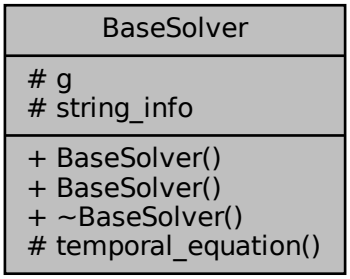
Base Solver for Gross Piteavskill finite difference solver.

`#include <base_solver.h>`

Inheritance diagram for BaseSolver:



Collaboration diagram for BaseSolver:



Public Member Functions

- BaseSolver ()=default
- BaseSolver (float g)

  Construct a new Base Solver:: Base Solver object.
- ~BaseSolver ()

  Destroy the Base Solver:: Base Solver object.

Protected Member Functions

- std::complex< float > temporal_equation (int i, int j, int k)

  defualt temporal equation

Protected Attributes

- float g
- std::string string_info

4.3.1 Detailed Description

Base Solver for Gross Piteavskill finite difference solver.

Definition at line 22 of file base_solver.h.

4.3.2 Constructor & Destructor Documentation

4.3.2.1 BaseSolver() [1/2]

```
BaseSolver::BaseSolver ( )  [default]
```

4.3.2.2 BaseSolver() [2/2]

```
BaseSolver::BaseSolver (
            float g_ )
```

Construct a new Base Solver:: Base Solver object.

Parameters

g_↩	

Definition at line 18 of file base_solver.cpp.

```
19     : g(g_){
20         this -> string_info = "Base_Solver";
21     };
```

4.3.2.3 ~BaseSolver()

```
BaseSolver::~BaseSolver ( )
```

Destroy the Base Solver:: Base Solver object.

Definition at line 28 of file base_solver.cpp.

```
28 {};
```

4.3.3 Member Function Documentation

4.3.3.1 temporal_equation()

```
std::complex< float > BaseSolver::temporal_equation (
            int i,
            int j,
            int k )  [protected]
```

defualt temporal equation

Returns

std::complex<float> 0+0i

Definition at line 36 of file base_solver.cpp.

```
36                                                          {
37     return std::complex<float> {0};
38 }
```

4.3.4 Member Data Documentation

4.3.4.1 g

```
float BaseSolver::g  [protected]
```

Definition at line 30 of file base_solver.h.

4.3.4.2 string_info

```
std::string BaseSolver::string_info  [protected]
```

Definition at line 32 of file base_solver.h.

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

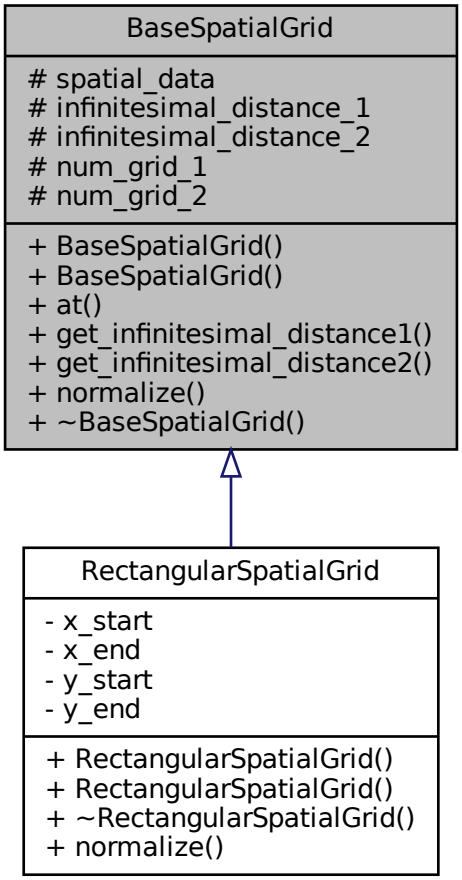
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/solver/base_solver.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/solver/base_solver.cpp

4.4 BaseSpatialGrid Class Reference

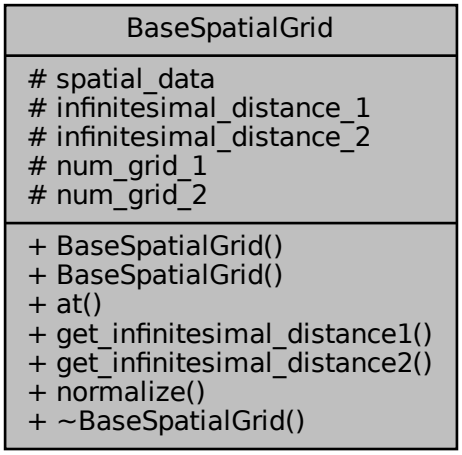
Base Spatial Grid class for single time step.

```
#include <base_domain.h>
```

Inheritance diagram for BaseSpatialGrid:



Collaboration diagram for BaseSpatialGrid:



Public Member Functions

- BaseSpatialGrid ()=default
- BaseSpatialGrid (int num_grid_1, int num_grid_2)
- GridPoint * at (int index_1, int index_2)
- float get_infinitesimal_distance1 ()
- float get_infinitesimal_distance2 ()
- void normalize ()
- ~BaseSpatialGrid ()

Protected Attributes

- std::vector< std::vector< GridPoint > > spatial_data
- float infinitesimal_distance_1
- float infinitesimal_distance_2
- int num_grid_1
- int num_grid_2

4.4.1 Detailed Description

Base Spatial Grid class for single time step.

Definition at line 46 of file base_domain.h.

4.4.2 Constructor & Destructor Documentation

4.4.2.1 BaseSpatialGrid() [1/2]

```
BaseSpatialGrid::BaseSpatialGrid ( )  [default]
```

4.4.2.2 BaseSpatialGrid() [2/2]

```
BaseSpatialGrid::BaseSpatialGrid (
            int num_grid_1,
            int num_grid_2 )
```

Definition at line 16 of file base_domain.cpp.

```
17 {
18     this->num_grid_1 = num_grid_1;
19     this->num_grid_2 = num_grid_2;
20     //Spatial_data: 2D matrix of grid points
21     this->spatial_data = std::vector<std::vector<GridPoint»(num_grid_1);
22     for (auto i = 0; i < num_grid_1; ++i)
23     {
24         this->spatial_data[i] = std::vector<GridPoint>(num_grid_2);
25     }
26     this-> infinitesimal_distance_1 = 1.f;
27     this -> infinitesimal_distance_2 = 1.f;
28 }
```

4.4.2.3 ~BaseSpatialGrid()

```
BaseSpatialGrid::~BaseSpatialGrid ( )
```

Definition at line 51 of file base_domain.cpp.

```
52 {
53
54     for (auto i = 0; i < num_grid_1; ++i)
55     {
56         this->spatial_data[i].clear();
57         std::vector<GridPoint>().swap(this->spatial_data[i]);
58     }
59     this->spatial_data.clear();
60     std::vector<std::vector<GridPoint»().swap(this->spatial_data);
61 }
```

4.4.3 Member Function Documentation

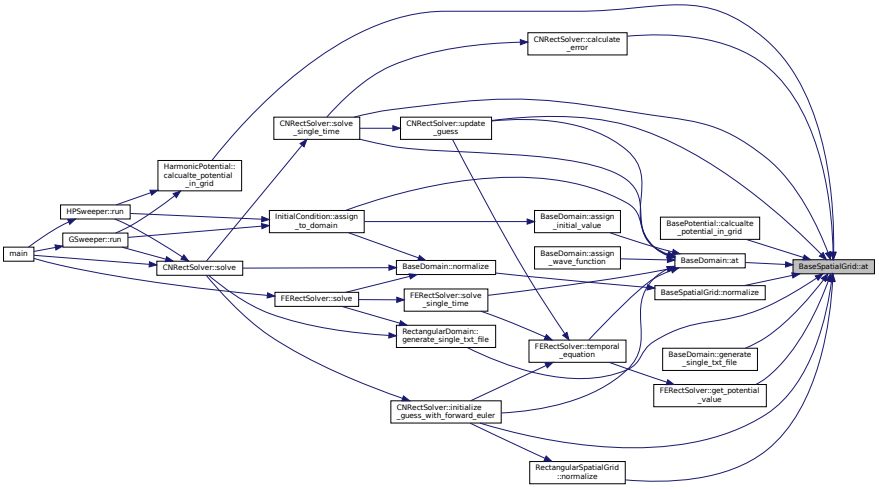
4.4.3.1 at()

```
GridPoint * BaseSpatialGrid::at (
            int index_1,
            int index_2 )
```

Definition at line 76 of file base_domain.cpp.

```
77 {
78     return &this->spatial_data[index_1 % this->num_grid_1][index_2 % this->num_grid_2];
79 }
```

Here is the caller graph for this function:



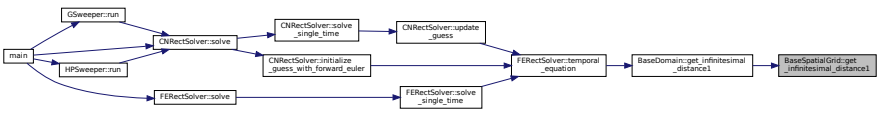
4.4.3.2 get_infinitesimal_distance1()

```
float BaseSpatialGrid::get_infinitesimal_distance1 ( )
```

Definition at line 64 of file base_domain.cpp.

```
65 {
66     return this->infinitesimal_distance_1;
67 }
```

Here is the caller graph for this function:



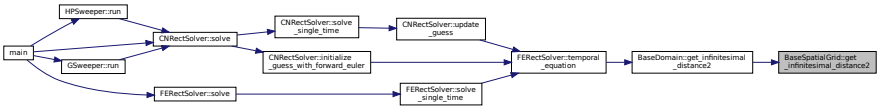
4.4.3.3 get_infinitesimal_distance2()

```
float BaseSpatialGrid::get_infinitesimal_distance2 ( )
```

Definition at line 70 of file base_domain.cpp.

```
71 {
72     return this->infinitesimal_distance_2;
73 }
```

Here is the caller graph for this function:



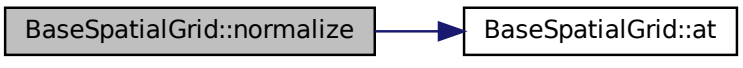
4.4.3.4 normalize()

```
void BaseSpatialGrid::normalize ( )
```

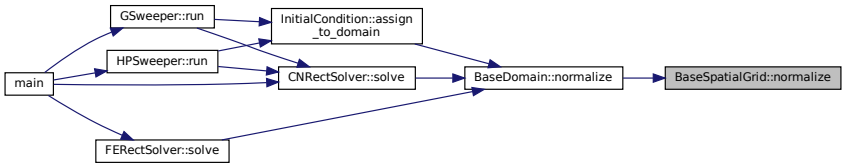
Definition at line 30 of file base_domain.cpp.

```
31 {
32     float sum = 0.;
33     for (auto i = 0; i < this->num_grid_1; ++i)
34     {
35         for (auto j = 0; j < this->num_grid_2; ++j)
36         {
37             auto wave_func = this->at(i, j)->value;
38             sum += float(std::pow(std::abs(wave_func), 2));
39         }
40     }
41     sum = std::sqrt(sum * this->infinitesimal_distance_1 * this->infinitesimal_distance_2);
42     for (auto i = 0; i < this->num_grid_1; ++i)
43     {
44         for (auto j = 0; j < this->num_grid_2; ++j)
45         {
46             this->at(i, j)->value /= sum;
47         }
48     }
49
50 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.4.4 Member Data Documentation

4.4.4.1 infinitesimal_distance_1

```
float BaseSpatialGrid::infinitesimal_distance_1  [protected]
```

Definition at line 59 of file base_domain.h.

4.4.4.2 infinitesimal_distance_2

```
float BaseSpatialGrid::infinitesimal_distance_2  [protected]
```

Definition at line 59 of file base_domain.h.

4.4.4.3 num_grid_1

```
int BaseSpatialGrid::num_grid_1  [protected]
```

Definition at line 60 of file base_domain.h.

4.4.4.4 num_grid_2

```
int BaseSpatialGrid::num_grid_2  [protected]
```

Definition at line 60 of file base_domain.h.

4.4.4.5 spatial_data

```
std::vector<std::vector<GridPoint> > BaseSpatialGrid::spatial_data  [protected]
```

Definition at line 58 of file base_domain.h.

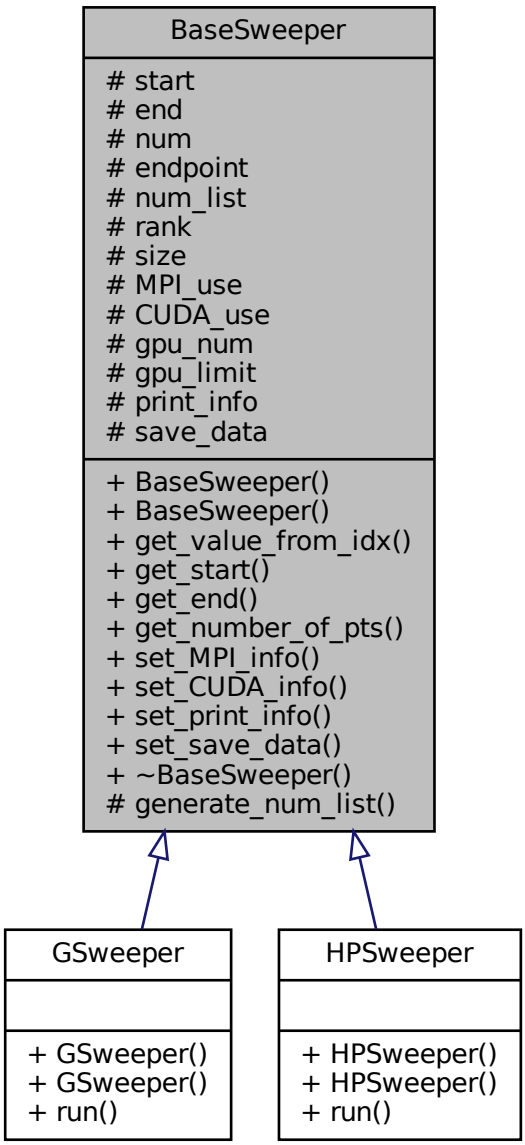
The documentation for this class was generated from the following files:

- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/domain/base_domain.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/domain/base_domain.cpp

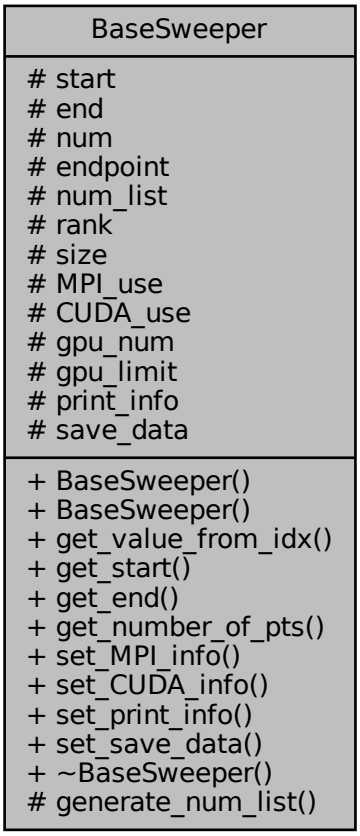
4.5 BaseSweeper Class Reference

```
#include <base_sweeper.h>
```

Inheritance diagram for BaseSweeper:



Collaboration diagram for BaseSweeper:



Public Member Functions

- BaseSweeper ()=default
- BaseSweeper (float start, float end, int num, bool endpoint=false)
- float get_value_from_idx (int idx)
- float get_start ()
- float get_end ()
- int get_number_of_pts ()
- virtual void set_MPI_info (int rank, int size)
- virtual void set_CUDA_info (int gpu_num, int gpu_limit)
- void set_print_info (bool print_info)
- void set_save_data (bool save_data)
- ~BaseSweeper ()

Protected Member Functions

- void generate_num_list ()

  generate number of points that sweep from start to end

Protected Attributes

- float start
- float end
- int num
- bool endpoint
- vector< float > num_list
- int rank =0
- int size =0
- bool MPI_use
- bool CUDA_use
- int gpu_num =1
- int gpu_limit =3
- bool print_info =true
- bool save_data =true

4.5.1 Detailed Description

Definition at line 7 of file base_sweeper.h.

4.5.2 Constructor & Destructor Documentation

4.5.2.1 BaseSweeper() [1/2]

```
BaseSweeper::BaseSweeper ( )  [default]
```

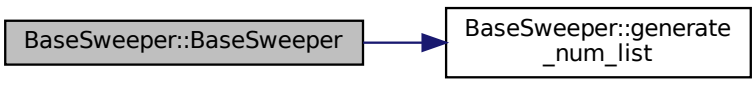
4.5.2.2 BaseSweeper() [2/2]

```
BaseSweeper::BaseSweeper (
            float start,
            float end,
            int num,
            bool endpoint = false )
```

Definition at line 5 of file base_sweeper.cpp.

```
5                                                                                   :
6 start(start_), end(end_), num(num_), endpoint(endpoint_){
7
8     this->generate_num_list();
9
10 }
```

Here is the call graph for this function:



4.5.2.3 ~BaseSweeper()

```
BaseSweeper::~BaseSweeper ( )
```

Definition at line 63 of file base_sweeper.cpp.

```
63 {};
```

4.5.3 Member Function Documentation

4.5.3.1 generate_num_list()

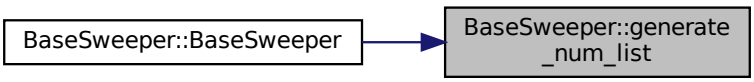
```
void BaseSweeper::generate_num_list ( )  [protected]
```

generate number of points that sweep from start to end

Definition at line 15 of file base_sweeper.cpp.

```
15                                          {
16     this->num_list = std::vector<float>(this->num);
17     float d = 0.;
18     if(this->endpoint){
19         d = (this -> end - this-> start ) / float(this-> num -1 );
20     }else{
21         d = (this -> end - this-> start ) / float(this-> num);
22     }
23
24     for (int i=0; i<this -> num; ++i){
25         this->num_list[i] = this ->start + d*i;
26     }
27
28 }
```

Here is the caller graph for this function:



4.5.3.2 get_end()

```
float BaseSweeper::get_end ( )
```

Definition at line 38 of file base_sweeper.cpp.

```
38                                  {
39     return end;
40 }
```

4.5.3.3 get_number_of_pts()

```
int BaseSweeper::get_number_of_pts ( )
```

Definition at line 41 of file base_sweeper.cpp.

```
41                                      {
42     return num;
43 }
```

4.5.3.4 get_start()

```
float BaseSweeper::get_start ( )
```

Definition at line 35 of file base_sweeper.cpp.

```
35                                  {
36     return start;
37 }
```

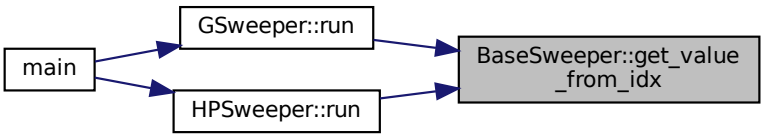
4.5.3.5 get_value_from_idx()

```
float BaseSweeper::get_value_from_idx (
            int idx )
```

Definition at line 31 of file base_sweeper.cpp.

```
31                                                  {
32     return this->num_list[idx];
33 }
```

Here is the caller graph for this function:



4.5.3.6 set_CUDA_info()

```
void BaseSweeper::set_CUDA_info (
            int gpu_num,
            int gpu_limit )  [virtual]
```

Definition at line 51 of file base_sweeper.cpp.

```
51                                                      {
52     this -> CUDA_use=true;
53     this -> gpu_num = gpu_num;
54     this -> gpu_limit = gpu_limit;
55 }
```

Here is the caller graph for this function:

4.5.3.7 set_MPI_info()

```
void BaseSweeper::set_MPI_info (
            int rank,
            int size )  [virtual]
```

Definition at line 45 of file base_sweeper.cpp.

```
45                                                  {
46     this -> rank = rank;
47     this -> size = size;
48     this -> MPI_use=true;
49 }
```

Here is the caller graph for this function:

4.5.3.8 set_print_info()

```
void BaseSweeper::set_print_info (
            bool print_info )
```

Definition at line 57 of file base_sweeper.cpp.

```
57                                                  {
58     this -> print_info = print_info;
59 }
```

Here is the caller graph for this function:

4.5.3.9 set_save_data()

```
void BaseSweeper::set_save_data (
            bool save_data )
```

Definition at line 60 of file base_sweeper.cpp.

```
60                                                  {
61     this -> save_data = save_data;
62 }
```

Here is the caller graph for this function:

4.5.4 Member Data Documentation

4.5.4.1 CUDA_use

```
bool BaseSweeper::CUDA_use  [protected]
```

Definition at line 36 of file base_sweeper.h.

4.5.4.2 end

```
float BaseSweeper::end  [protected]
```

Definition at line 25 of file base_sweeper.h.

4.5.4.3 endpoint

```
bool BaseSweeper::endpoint  [protected]
```

Definition at line 27 of file base_sweeper.h.

4.5.4.4 gpu_limit

```
int BaseSweeper::gpu_limit =3  [protected]
```

Definition at line 38 of file base_sweeper.h.

4.5.4.5 gpu_num

```
int BaseSweeper::gpu_num =1  [protected]
```

Definition at line 37 of file base_sweeper.h.

4.5.4.6 MPI_use

```
bool BaseSweeper::MPI_use  [protected]
```

Definition at line 34 of file base_sweeper.h.

4.5.4.7 num

```
int BaseSweeper::num  [protected]
```

Definition at line 26 of file base_sweeper.h.

4.5.4.8 num_list

```
vector<float> BaseSweeper::num_list  [protected]
```

Definition at line 28 of file base_sweeper.h.

4.5.4.9 print_info

```
bool BaseSweeper::print_info =true  [protected]
```

Definition at line 40 of file base_sweeper.h.

4.5.4.10 rank

```
int BaseSweeper::rank =0  [protected]
```

Definition at line 32 of file base_sweeper.h.

4.5.4.11 save_data

```
bool BaseSweeper::save_data =true  [protected]
```

Definition at line 41 of file base_sweeper.h.

4.5.4.12 size

```
int BaseSweeper::size =0  [protected]
```

Definition at line 33 of file base_sweeper.h.

4.5.4.13 start

```
float BaseSweeper::start  [protected]
```

Definition at line 24 of file base_sweeper.h.

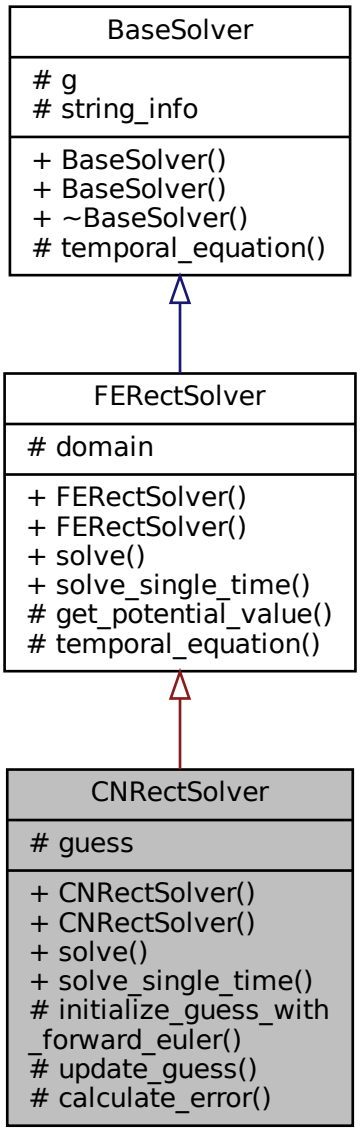
The documentation for this class was generated from the following files:

- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/sweeper/base_sweeper.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/sweeper/base_sweeper.cpp

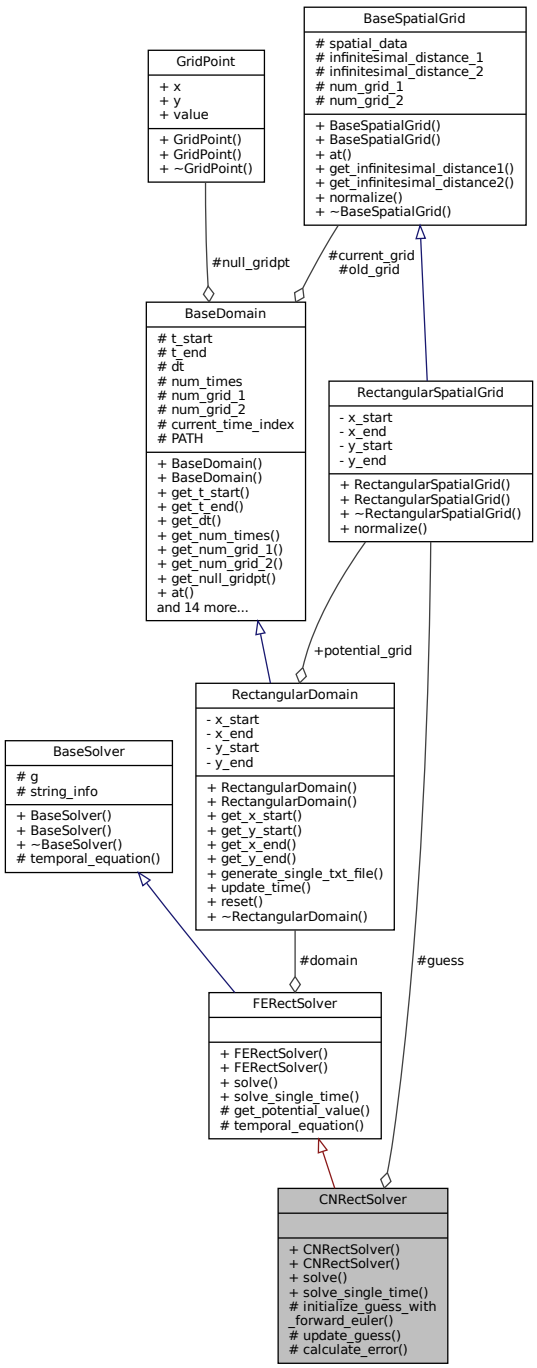
4.6 CNRectSolver Class Reference

`#include <cn_rect_solver.h>`

Inheritance diagram for CNRectSolver:



Collaboration diagram for CNRectSolver:



Public Member Functions

- CNRectSolver ()=default
- CNRectSolver (float g, RectangularDomain ∗domain)

  Construct a new CNRectSolver::CNRectSolver object.
- void solve (float tolerance, int max_iter, std::string dir_name="", bool print_info=true, bool save_data=true)

  solve equation with crank nicolson method with given max_iter and tolerance.

- void solve_single_time (int k, float tolerance, int max_iter)
  Solve spatial domain for temporal index k.

Protected Member Functions

- void initialize_guess_with_forward_euler (int k)
  initialize guess with forward euler method
- void update_guess (int i, int j, int k)
  Update guess of the spatial(i, j), temporal k point.
- float calculate_error (int k)
  Calculate L2 error between the ccurrent and previous guess.

Protected Attributes

- RectangularSpatialGrid * guess

Private Member Functions

- void solve (std::string dir_name="", bool print_info=true, bool save_data=true)
  Solve Equation.
- void solve_single_time (int k)
  Update k+1 th wave function value with k th values.
- float get_potential_value (int i, int j)
  Get Potential value on each grid point.
- std::complex< float > temporal_equation (int i, int j, int k)
  Time differential of phi.

Private Attributes

- RectangularDomain * domain
- float g
- std::string string_info

4.6.1 Detailed Description

Definition at line 24 of file cn_rect_solver.h.

4.6.2 Constructor & Destructor Documentation

4.6.2.1 CNRectSolver() [1/2]

```
CNRectSolver::CNRectSolver ( )  [default]
```

4.6.2.2 CNRectSolver() [2/2]

```
CNRectSolver::CNRectSolver (
            float g,
            RectangularDomain * domain )
```

Construct a new CNRectSolver::CNRectSolver object.

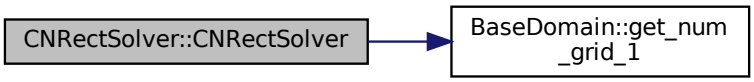
Parameters

g	
domain	

Definition at line 20 of file cn_rect_solver.cpp.

```
23     : FERectSolver(g, domain) //
24 {
25     // this->generate_potential_grid();
26     this->guess = new RectangularSpatialGrid(
27         this->domain->get_num_grid_1(),
28         this->domain->get_num_grid_2(),
29         this->domain->get_x_start(),
30         this->domain->get_x_end(),
31         this->domain->get_y_start(),
32         this->domain->get_y_end());
33     this->string_info = std::string{"Crank_Nicolson_serial_"};
34 };
```

Here is the call graph for this function:



4.6.3 Member Function Documentation

4.6.3.1 calculate_error()

```
float CNRectSolver::calculate_error (
            int k )  [protected]
```

Calculate L2 error between the ccurrent and previous guess.

Parameters

k	

Returns

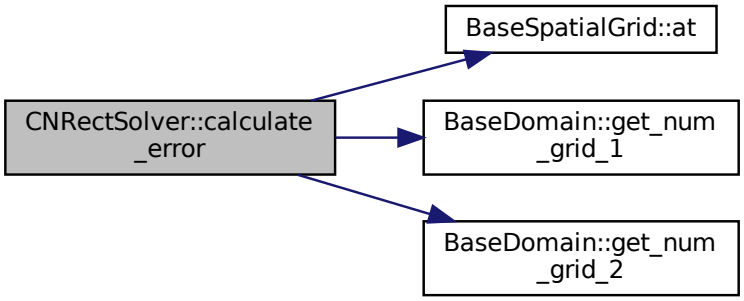
float

Definition at line 94 of file cn_rect_solver.cpp.

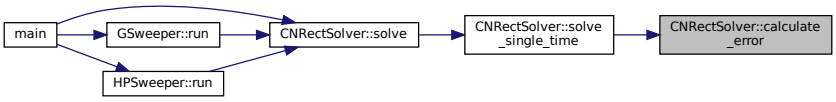
```
95 {
96     float error = 0.;
97     for (auto i = 0; i < this->domain->get_num_grid_1(); ++i)
98     {
99         for (auto j = 0; j < this->domain->get_num_grid_2(); ++j)
```

```
100         {
101             error += std::pow(std::abs((this->guess->at(i, j)->value - this->domain->at(i, j,
        k)->value)), 2);
102         }
103      }
104      return error;
105 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.6.3.2 get_potential_value()

```
float FERectSolver::get_potential_value (
            int i,
            int j )  [protected], [inherited]
```

Get Potential value on each grid point.

Parameters

i	
j	

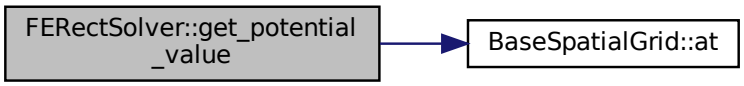
Returns

float

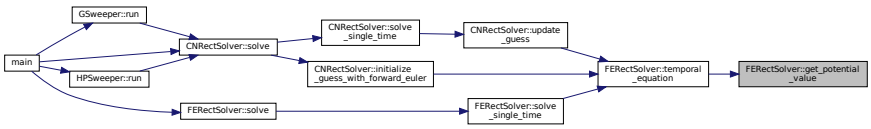
Definition at line 37 of file fe_rect_solver.cpp.

```
38 {
39
40     return this->domain->potential_grid->at(i, j)->value.real();
41 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.6.3.3 initialize_guess_with_forward_euler()

```
void CNRectSolver::initialize_guess_with_forward_euler (
            int k )  [protected]
```

initialize guess with forward euler method

Parameters

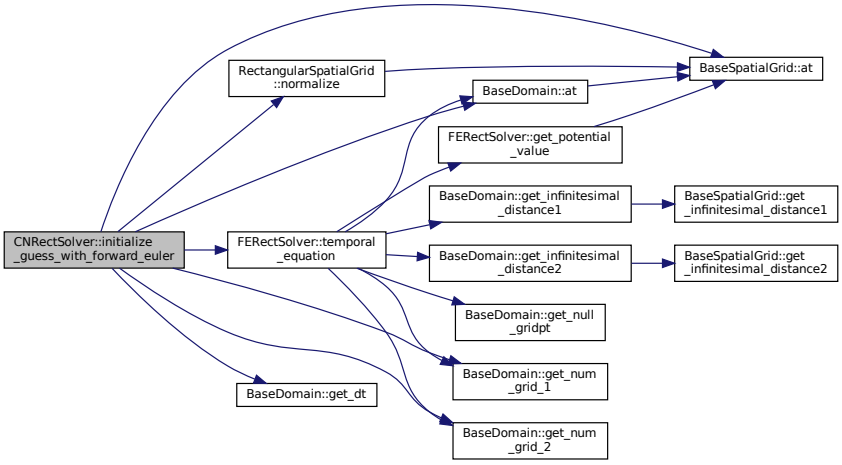
k	

Definition at line 41 of file cn_rect_solver.cpp.

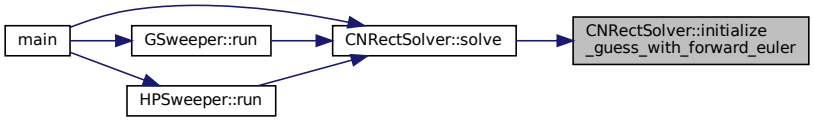
```
42 {
43     delete this->guess;
44     this->guess = new RectangularSpatialGrid(
45         this->domain->get_num_grid_1(),
46         this->domain->get_num_grid_2(),
47         this->domain->get_x_start(),
48         this->domain->get_x_end(),
49         this->domain->get_y_start(),
50         this->domain->get_y_end());
51     for (auto i = 0; i < this->domain->get_num_grid_1(); ++i)
52     {
53         for (auto j = 0; j < this->domain->get_num_grid_2(); ++j)
```

```
54         {
55
56             //At first, initial guess is the results of fe algorithm
57             this->domain->at(i, j, k)->value = this->domain->at(i, j, k - 1)->value +
       this->domain->get_dt() * (this->temporal_equation(i, j, k - 1));
58             this->guess->at(i, j)->value = this->domain->at(i, j, k)->value;
59         }
60     }
61     this -> guess ->normalize();
62 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.6.3.4 solve() [1/2]

```
void CNRectSolver::solve (
            float tolerance,
            int max_iter,
            std::string dir_name = "",
            bool print_info = true,
            bool save_data = true )
```

solve equation with crank nicolson method with given max_iter and tolerance.

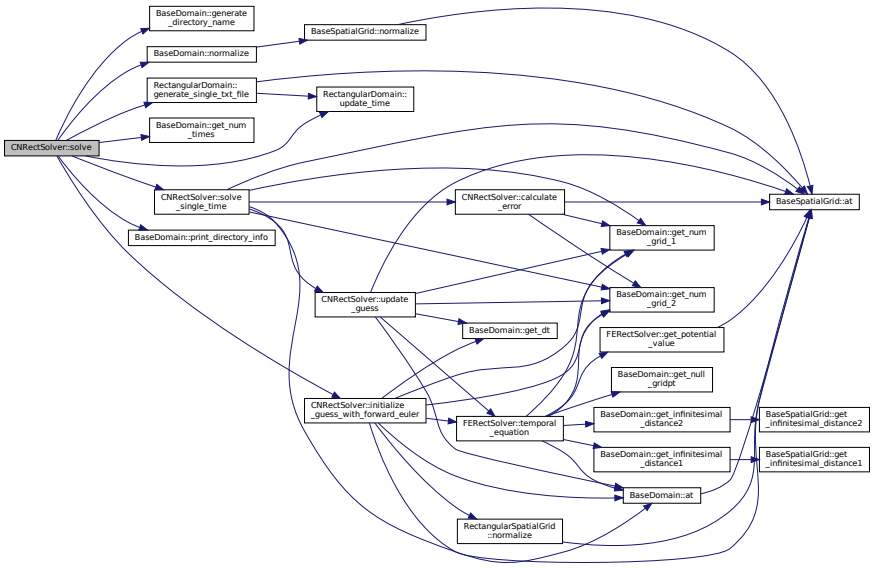
Parameters

tolerance	
max_iter	
dir_name	
print_info	
save_data	

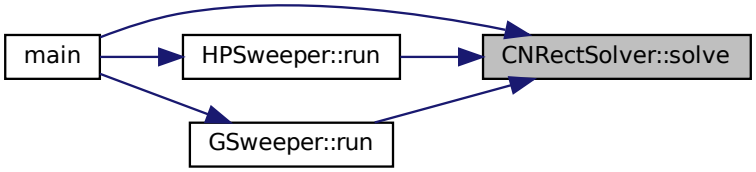
Definition at line 162 of file cn_rect_solver.cpp.

```
163 {
164     int time_length = this->domain->get_num_times();
165     //Save initial condition at time = start_time
166     if(save_data){
167         this->domain->generate_directory_name(this->string_info+dir_name, print_info);
168         //Save initial condition
169         this->domain->generate_single_txt_file(std::string("Solution_") + std::to_string(0));
170     }else{
171         this -> domain->update_time();
172     }
173     for (int k = 0; k < time_length-1; ++k)
174     {
175         //Update kth grid using k-1 th grid
176         // std::cout « "time step " « k « std::endl;
177 
178         this->initialize_guess_with_forward_euler(k+1);
179         this->solve_single_time(k+1, tolerance, max_iter);
180         this->domain->normalize(k+1);
181         if(save_data){
182             this->domain->generate_single_txt_file(std::string("Solution_") + std::to_string(k+1));
183         }
184         else{
185             this->domain->update_time();
186         }
187     }
188     if(print_info){
189         this->domain->print_directory_info();
190     }
191 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.6.3.5 solve() [2/2]

```
void FERectSolver::solve (
            std::string dir_name = "",
            bool print_info = true,
            bool save_data = true )  [inherited]
```

Solve Equation.

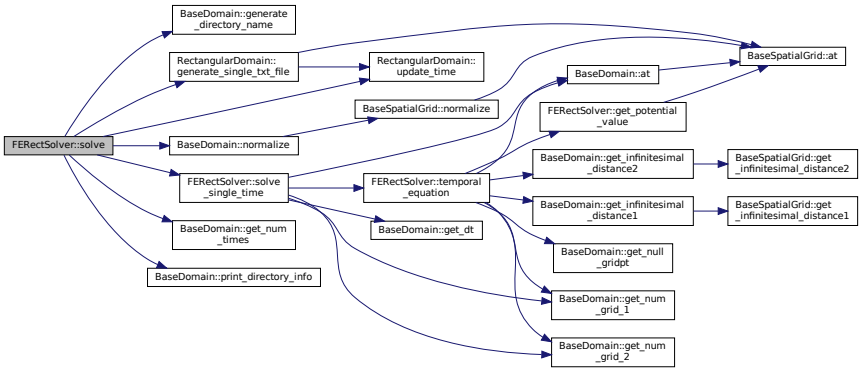
Parameters

dir_name	
print_info	
save_data	

Definition at line 116 of file fe_rect_solver.cpp.

```
117 {
118     int time_length = this->domain->get_num_times();
119     if(save_data){
120         this->domain->generate_directory_name(this->string_info+dir_name, print_info);
121         //Save initial condition
122         this->domain->generate_single_txt_file(std::string("Solution_") + std::to_string(0));
123     }else{
124         this -> domain->update_time();
125     }
126
127     for (int k = 0; k < time_length - 1; ++k)
128     {
129         this->solve_single_time(k);
130         this->domain->normalize(k + 1);
131         if(save_data){
132             this->domain->generate_single_txt_file(std::string("Solution_") + std::to_string(k + 1));
133         }
134         else{
135             this->domain->update_time();
136         }
137     }
138     if(print_info){
139         this->domain->print_directory_info();
140     }
141 }
```

Here is the call graph for this function:



Here is the caller graph for this function:

4.6.3.6 solve_single_time() [1/2]

```
void FERectSolver::solve_single_time (
            int k )  [inherited]
```

Update k+1 th wave function value with k th values.

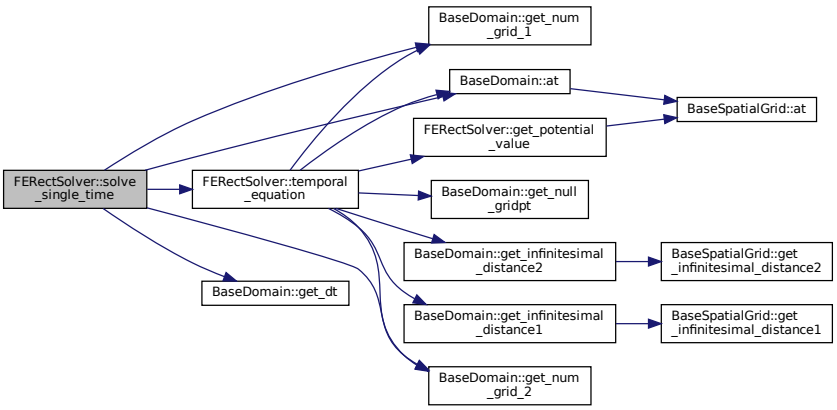
Parameters

k	

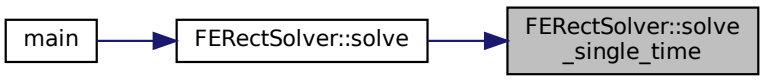
Definition at line 95 of file fe_rect_solver.cpp.

```
96 {
97     int Nx = this->domain->get_num_grid_1();
98     int Ny = this->domain->get_num_grid_2();
99     float dt = this->domain->get_dt();
100     for (int i = 0; i < Nx; ++i)
101     {
102         for (int j = 0; j < Ny; ++j)
103         {
104             (this->domain->at(i, j, k + 1)->value) = this->domain->at(i, j, k)->value + dt *
      this->temporal_equation(i, j, k);
105         }
106     }
107 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.6.3.7 solve_single_time() [2/2]

```
void CNRectSolver::solve_single_time (
            int k,
            float tolerance,
            int max_iter )
```

Solve spatial domain for temporal index k.

Parameters

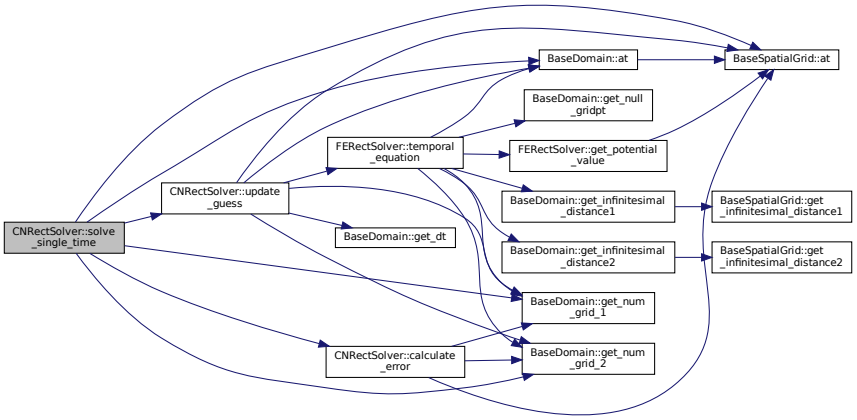
k	
tolerance	
max_iter	

Definition at line 114 of file cn_rect_solver.cpp.

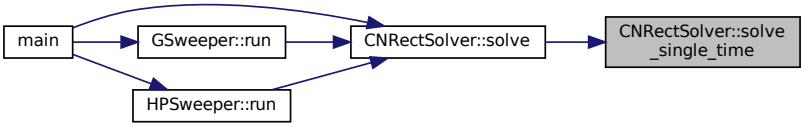
```
115 {
116     float error = 1.;
117     bool converged = false;
118     int converged_step = 0;
119     for (auto iter = 0; iter < max_iter; ++iter)
```

```
120     {
121         if (error < tolerance)
122         {
123             converged = true;
124             converged_step = iter - 1;
125             break;
126         }
127         //For each point, update wave function
128         for (auto i = 0; i < this->domain->get_num_grid_1(); ++i)
129         {
130             for (auto j = 0; j < this->domain->get_num_grid_2(); ++j)
131             {
132                 this->domain->at(i, j, k)->value = this->guess->at(i, j)->value;
133             }
134         }
135 
136         //for each point, update predicted value
137         for (auto i = 0; i < this->domain->get_num_grid_1(); ++i)
138         {
139             for (auto j = 0; j < this->domain->get_num_grid_2(); ++j)
140             {
141                 update_guess(i, j, k);
142             }
143         }
144         error = this->calculate_error(k);
145 
146     }
147     if (!converged)
148     {
149         std::cout « "At time "«k «" Converged failed with error = " « error « std::endl;
150     }
151 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.6.3.8 temporal_equation()

```
std::complex< float > FERectSolver::temporal_equation (
            int i,
            int j,
            int k )  [protected], [inherited]
```

Time differential of phi.

Parameters

i	index for x
j	index for y
k	index for time(t)

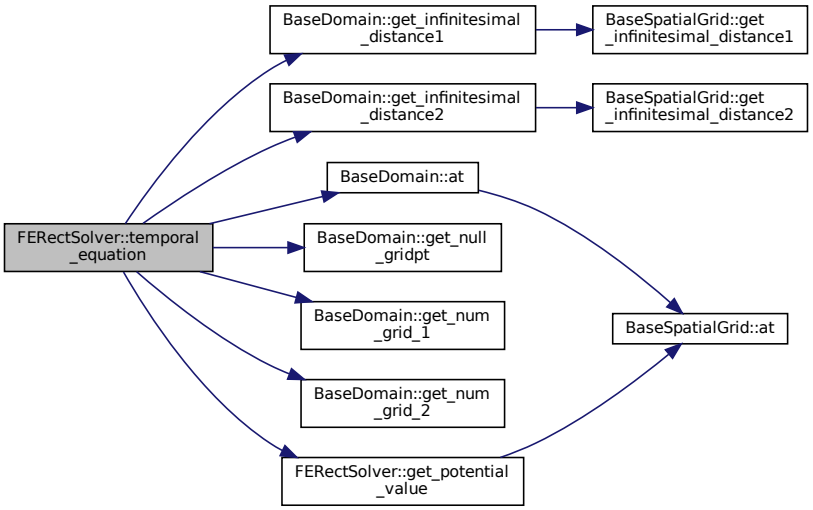
Returns

std::complex<float> time differential at x, y, t

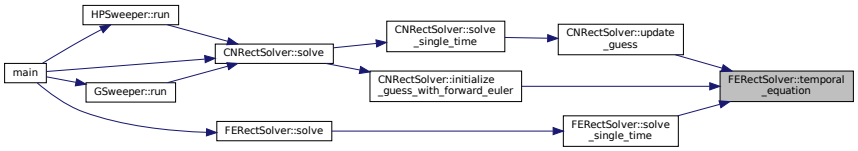
Definition at line 51 of file fe_rect_solver.cpp.

```
52 {
53     //Use five stencil method
54     auto point_data = this->domain->at(i, j, k);
55 
56     //l,r,d,u denotes left, right, down, up value
57     //Check boundary
58     auto point_data_l = this->domain->at(i - 1, j, k);
59     if (i <= 0)
60         point_data_l = this->domain->get_null_gridpt();
61     auto point_data_d = this->domain->at(i, j - 1, k);
62     if (j <= 0)
63         point_data_d = this->domain->get_null_gridpt();
64     auto point_data_r = this->domain->at(i + 1, j, k);
65     if (i >= (this->domain->get_num_grid_1()) - 1)
66         point_data_r = this->domain->get_null_gridpt();
67     auto point_data_u = this->domain->at(i, j + 1, k);
68     if (j >= (this->domain->get_num_grid_2()) - 1)
69         point_data_u = this->domain->get_null_gridpt();
70 
71     //potential at x, y
72     float V_ij = this->get_potential_value(i, j);
73     //this->potential_func(point_data->x, point_data->y);
74 
75     //g * |psi(x,y)|^2
76     float additional_term = (this->g) * (std::abs(point_data->value)) * (std::abs(point_data->value));
77 
78     //Set infinitesimal value
79     float dx = this->domain->get_infinitesimal_distance1();
80     float dy = this->domain->get_infinitesimal_distance2();
81     //df denote time differential of dt (d(psi)/dt)
82     // = (laplace - V-g|psi|^2) psi
83     std::complex<float> df =
84         +((point_data_r->value) + (point_data_l->value) - (point_data->value) * std::complex<float>{2}) /
       (std::complex<float>{dx * dx}) + ((point_data_u->value) + (point_data_d->value) - (point_data->value)
       * std::complex<float>{2}) / (std::complex<float>{dy * dy}) - (V_ij + additional_term) *
       (point_data->value);
85     df *= std::complex<float>{0, 1};
86 
87     return df;
88 };
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.6.3.9 update_guess()

```
void CNRectSolver::update_guess (
            int i,
            int j,
            int k )  [protected]
```

Update guess of the spatial(i, j), temporal k point.

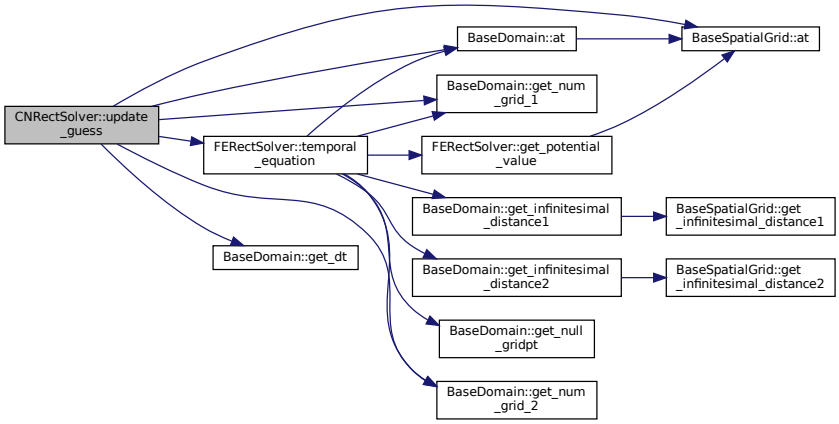
Parameters

i	
j	
k	

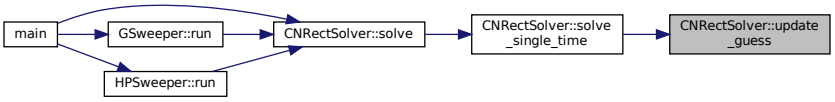
Definition at line 71 of file cn_rect_solver.cpp.

```
72 {
73     for (auto i = 0; i < this->domain->get_num_grid_1(); ++i)
74     {
75         for (auto j = 0; j < this->domain->get_num_grid_2(); ++j)
76         {
77             this->guess->at(i, j)->value = (
78                 0.99f * this->guess->at(i, j)->value +
79                 0.01f * (
80                     this->domain->at(i, j, k - 1)->value +
81                     std::complex<float>{0.5, 0.} * this->domain->get_dt() * (
82                         this->temporal_equation(i, j, k - 1) +
83                         this->temporal_equation(i, j, k)))); // this->temporal_equation_from_guess(i,
    j))));
84         }
85     }
86 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.6.4 Member Data Documentation

4.6.4.1 domain

```
RectangularDomain* FERectSolver::domain  [protected], [inherited]
```

Definition at line 39 of file fe_rect_solver.h.

4.6.4.2 g

```
float BaseSolver::g  [protected], [inherited]
```

Definition at line 30 of file base_solver.h.

4.6.4.3 guess

```
RectangularSpatialGrid* CNRectSolver::guess  [protected]
```

Definition at line 35 of file cn_rect_solver.h.

4.6.4.4 string_info

```
std::string BaseSolver::string_info  [protected], [inherited]
```

Definition at line 32 of file base_solver.h.

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

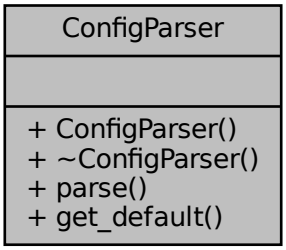
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/solver/serial_solver/crank_nicolson/cn_rect_solver.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/solver/serial_solver/crank_nicolson/cn_rect_solver.cpp

4.7 ConfigParser Class Reference

Configuration parser.

```
#include <config_parser.h>
```

Collaboration diagram for ConfigParser:



Public Member Functions

- ConfigParser ()=default
- virtual ~ConfigParser ()=default

Static Public Member Functions

- static Parameters parse (std::string config_name, std::string filename)

  Parse configuration for the calculation.
- static Parameters get_default ()

  Setup parameters with default values.

4.7.1 Detailed Description

Configuration parser.

Definition at line 27 of file config_parser.h.

4.7.2 Constructor & Destructor Documentation

4.7.2.1 ConfigParser()

```
ConfigParser::ConfigParser ( )  [default]
```

4.7.2.2 ~ConfigParser()

```
virtual ConfigParser::~ConfigParser ( )  [virtual], [default]
```

4.7.3 Member Function Documentation

4.7.3.1 get_default()

```
Parameters ConfigParser::get_default ( )  [static]
```

Setup parameters with default values.

Returns

Parameters

Definition at line 494 of file config_parser.cpp.

```
495 {
496     auto parameters = Parameters();
497     parameters.config_name = "default";
498     MainParameters main_parameters;
499     DomainParameters domain_parameters;
500     InitialConditionParameters init_parameters;
501     EquationParameters equation_parameters;
502     SolverParameters solver_parameters;
503 
504     main_parameters.calculation_type = "single";
505     domain_parameters.domain_type = "rectangular";
506     domain_parameters.n_x = 256;
507     domain_parameters.n_y = 256;
508     domain_parameters.n_time = 5;
509     domain_parameters.time_start = 0.;
510     domain_parameters.time_end = 0.01;
511     domain_parameters.spatial_parameters["x_start"] = -10.;
512     domain_parameters.spatial_parameters["x_end"] = 10.;
513     domain_parameters.spatial_parameters["y_start"] = -10.;
514     domain_parameters.spatial_parameters["y_end"] = 10.;
515 
516     init_parameters.init_cond_type = "singlegaussian";
517     init_parameters.init_cond_parameters["sigma_x"] = 1.;
518     init_parameters.init_cond_parameters["sigma_y"] = 1.;
519     init_parameters.init_cond_parameters["center_x"] = 0.;
520     init_parameters.init_cond_parameters["center_y"] = 0.;
521 
522     equation_parameters.potential_type = "harmonic";
523     equation_parameters.g = -1;
524     equation_parameters.potential_parameters["omega_x"] = 3.;
525     equation_parameters.potential_parameters["omega_y"] = 5.;
526 
527     solver_parameters.method = "cranknicolson";
528     solver_parameters.run_parallel = true;
529     solver_parameters.print_info = false;
530     solver_parameters.save_data = false;
531     solver_parameters.solver_parameters["converge_crit"] = 1e-11;
532     solver_parameters.int_parameters["max_iter"] = 1001;
533     solver_parameters.int_parameters["cuda_device"] = 0;
534 
535     parameters.main_parameters = main_parameters;
536     parameters.domain_parameters = domain_parameters;
537     parameters.init_cond_parameters = init_parameters;
538     parameters.equation_parameters = equation_parameters;
539     parameters.solver_parameters = solver_parameters;
540     return parameters;
541 }
```

Here is the caller graph for this function:

4.7.3.2 parse()

```
Parameters ConfigParser::parse (
            std::string config_name,
            std::string filename )  [static]
```

Parse configuration for the calculation.

Parameters

config_name	configuration name
filename	configuration file name

Returns

Parsed parameters

Definition at line 21 of file config_parser.cpp.

```
21                                                                                  {
22     auto parameters = Parameters();
23     parameters.config_name = config_name;
24     // -1 for outside, 0 for main,  1 for domain, 2 for initial condition, 3 for eqution, 4 for solver
25     int mode = -1;
26     MainParameters main_parameters;
27     DomainParameters domain_parameters;
28     InitialConditionParameters init_parameters;
29     EquationParameters equation_parameters;
30     SolverParameters solver_parameters;
31     bool filled_parallel = false;
32 
33     std::ifstream file(filename.c_str());
34     if (file.is_open()) // If file is opened
35     {
36         std::string line;
37         while (std::getline(file, line)) // while not EOF
38         {
39             // remove all blanks in the line
40             line.erase(std::remove(line.begin(), line.end(), ' '), line.end());
41             // replace all lines with lower case
42             std::transform(line.begin(), line.end(), line.begin(),
43                            [](unsigned char c)
44                            { return std::tolower(c); });
45 
46             // skip the line when whole line is blank
47             if (line == ""){
48                 continue;
49             }
50             // skip the line for the comment
51             else if (line.rfind("#", 0) != std::string::npos)
52             {
53                 continue;
54             }
55             // Divide the configuration branches (0 for main,  1 for domain, 2 for initial condition, 3
    for eqution, 4 for solver)
56             else if (line.rfind("[mainconfiguration]", 0) != std::string::npos)
57             {
58                 mode = 0;
59             }
60             else if (line.rfind("[domainconfiguration]", 0) != std::string::npos)
61             {
62                 mode = 1;
63             }
64             else if (line.rfind("[initialconditionconfiguration]", 0) != std::string::npos)
65             {
66                 mode = 2;
67             }
68             else if (line.rfind("[equationconfiguration]", 0) != std::string::npos)
69             {
70                 mode = 3;
71             }
72             else if (line.rfind("[solverconfiguration]", 0) != std::string::npos)
73             {
74                 mode = 4;
75             }
```

```
76              // Do action for each branches
77              else{
78                  // Handle exception
79                  if (mode == -1){
80                      std::cerr « "Unexpected Configuration File" « std::endl;
81                  }
82                  // Main branch
83                  else if(mode == 0){
84                      std::vector<std::string> dump;
85                      std::string tmp;
86                      std::stringstream string_stream(line);
87                      if (line.rfind("type", 0) != std::string::npos)
88                      {
89                          while (std::getline(string_stream, tmp, '='))
90                          {
91                              dump.push_back(tmp);
92                          }
93                          if (dump.size() != 2)
94                          {
95                              std::cerr « "Unexpected Configuration File" « std::endl;
96                          }
97                          main_parameters.calculation_type = dump[1];
98                      }
99                      else{
100                          while (std::getline(string_stream, tmp, '='))
101                          {
102                              dump.push_back(tmp);
103                          }
104                          if (dump.size() != 2)
105                          {
106                              std::cerr « "Unexpected Configuration File" « std::endl;
107                          }
108                          if (dump[0] == "sweep_start")
109                          {
110                              main_parameters.float_parameters[dump[0]] =
    (float)std::atof(dump[1].c_str());
111                          }
112                          else if (dump[0] == "sweep_end")
113                          {
114                              main_parameters.float_parameters[dump[0]] =
    (float)std::atof(dump[1].c_str());
115                          }
116                          else if (dump[0] == "sweep_count")
117                          {
118                              main_parameters.int_parameters[dump[0]] = std::atoi(dump[1].c_str());
119                          }
120                          else if (dump[0] == "end_point")
121                          {
122                              if (dump[1] == "true")
123                              {
124                                  main_parameters.int_parameters[dump[0]] = (int)true;
125                              }
126                              else if (dump[1] == "false")
127                              {
128                                  main_parameters.int_parameters[dump[0]] = (int)false;
129                              }
130                              else
131                              {
132                                  std::cerr « "Unexpected Configuration File" « std::endl;
133                              }
134                          }
135                          else if (dump[0] == "mpi_use")
136                          {
137                              if (dump[1] == "true")
138                              {
139                                  main_parameters.int_parameters[dump[0]] = (int)true;
140                              }
141                              else if (dump[1] == "false")
142                              {
143                                  main_parameters.int_parameters[dump[0]] = (int)false;
144                              }
145                              else
146                              {
147                                  std::cerr « "Unexpected Configuration File" « std::endl;
148                              }
149                          }
150                          else if (dump[0] == "cuda_use")
151                          {
152                              if (dump[1] == "true")
153                              {
154                                  main_parameters.int_parameters[dump[0]] = (int)true;
155                              }
156                              else if (dump[1] == "false")
157                              {
158                                  main_parameters.int_parameters[dump[0]] = (int)false;
159                              }
160                              else
```

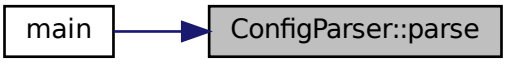
```
161                             {
162                                 std::cerr « "Unexpected Configuration File" « std::endl;
163                             }
164                         }
165                         else if (dump[0] == "gpu_count")
166                         {
167                             main_parameters.int_parameters[dump[0]] = std::atoi(dump[1].c_str());
168                         }
169                         else if (dump[0] == "calculation_per_gpu")
170                         {
171                             main_parameters.int_parameters[dump[0]] = std::atoi(dump[1].c_str());
172                         }
173                         else
174                         {
175                             std::cerr « "Unexpected Configuration File" « std::endl;
176                         }
177                     }
178                 }
179                 // domain branch
180                 else if(mode == 1){
181                     std::vector<std::string> dump;
182                     std::string tmp;
183                     std::stringstream string_stream(line);
184                     if (line.rfind("type", 0) != std::string::npos)
185                     {
186                         while (std::getline(string_stream, tmp, '='))
187                         {
188                             dump.push_back(tmp);
189                         }
190                         if (dump.size() != 2){
191                             std::cerr « "Unexpected Configuration File" « std::endl;
192                         }
193                         domain_parameters.domain_type = dump[1];
194                     }
195                     else{
196                         while (std::getline(string_stream, tmp, '='))
197                         {
198                             dump.push_back(tmp);
199                         }
200                         if (dump.size() != 2)
201                         {
202                             std::cerr « "Unexpected Configuration File" « std::endl;
203                         }
204 
205                         if (domain_parameters.domain_type != ""){
206                             while (std::getline(string_stream, tmp, '='))
207                             {
208                                 dump.push_back(tmp);
209                             }
210                             if (dump.size() != 2)
211                             {
212                                 std::cerr « "Unexpected Configuration File" « std::endl;
213                             }
214 
215                             if (dump[0] == "n_x"){
216                                 domain_parameters.n_x = std::atoi(dump[1].c_str());
217                             }
218                             else if(dump[0] == "n_y"){
219                                 domain_parameters.n_y = std::atoi(dump[1].c_str());
220                             }
221                             else if(dump[0] == "n_time"){
222                                 domain_parameters.n_time = std::atoi(dump[1].c_str());
223                             }
224                             else if(dump[0] == "time_start"){
225                                 domain_parameters.time_start = (float)std::atof(dump[1].c_str());
226                             }
227                             else if(dump[0] == "time_end"){
228                                 domain_parameters.time_end = (float)std::atof(dump[1].c_str());
229                             }
230                             else{
231                                 domain_parameters.spatial_parameters[dump[0]] =
    (float)std::atof(dump[1].c_str());
232                             }
233                         }
234                         else{
235                             std::cerr « "Unexpected Configuration File" « std::endl;
236                         }
237                     }
238                 }
239                 // initial condition branches
240                 else if(mode == 2){
241                     std::vector<std::string> dump;
242                     std::string tmp;
243                     std::stringstream string_stream(line);
244                     if (line.rfind("type", 0) != std::string::npos)
245                     {
246                         while (std::getline(string_stream, tmp, '='))
```

```
247                         {
248                             dump.push_back(tmp);
249                         }
250                         if (dump.size() != 2)
251                         {
252                             std::cerr « "Unexpected Configuration File" « std::endl;
253                         }
254                         init_parameters.init_cond_type = dump[1];
255                     }
256                     else
257                     {
258                         while (std::getline(string_stream, tmp, '='))
259                         {
260                             dump.push_back(tmp);
261                         }
262                         if (dump.size() != 2)
263                         {
264                             std::cerr « "Unexpected Configuration File" « std::endl;
265                         }
266 
267                         if (init_parameters.init_cond_type != "")
268                         {
269                             init_parameters.init_cond_parameters[dump[0]] =
    (float)std::atof(dump[1].c_str());
270                         }
271                         else
272                         {
273                             std::cerr « "Unexpected Configuration File" « std::endl;
274                         }
275                     }
276                 }
277                 // eqution branch
278                 else if(mode == 3){
279                     std::vector<std::string> dump;
280                     std::string tmp;
281                     std::stringstream string_stream(line);
282                     if (line.rfind("type", 0) != std::string::npos)
283                     {
284                         while (std::getline(string_stream, tmp, '='))
285                         {
286                             dump.push_back(tmp);
287                         }
288                         if (dump.size() != 2)
289                         {
290                             std::cerr « "Unexpected Configuration File" « std::endl;
291                         }
292                         equation_parameters.potential_type = dump[1];
293                     }
294                     else if (line.rfind("g", 0) != std::string::npos)
295                     {
296                         while (std::getline(string_stream, tmp, '='))
297                         {
298                             dump.push_back(tmp);
299                         }
300                         if (dump.size() != 2)
301                         {
302                             std::cerr « "Unexpected Configuration File" « std::endl;
303                         }
304                         equation_parameters.g = std::atof(dump[1].c_str());
305                     }
306                     else
307                     {
308                         while (std::getline(string_stream, tmp, '='))
309                         {
310                             dump.push_back(tmp);
311                         }
312                         if (dump.size() != 2)
313                         {
314                             std::cerr « "Unexpected Configuration File" « std::endl;
315                         }
316 
317                         if (equation_parameters.potential_type != "")
318                         {
319                             equation_parameters.potential_parameters[dump[0]] =
    std::atof(dump[1].c_str());
320                         }
321                         else
322                         {
323                             std::cerr « "Unexpected Configuration File" « std::endl;
324                         }
325                     }
326                 }
327                 // solver branch
328                 else if (mode == 4){
329                     std::vector<std::string> dump;
330                     std::string tmp;
331                     std::stringstream string_stream(line);
```

```
332
333                     // Get Method
334                     if (line.rfind("method", 0) != std::string::npos)
335                     {
336                         while (std::getline(string_stream, tmp, '='))
337                         {
338                             dump.push_back(tmp);
339                         }
340                         if (dump.size() != 2)
341                         {
342                             std::cerr << "Unexpected Configuration File" << std::endl;
343                         }
344                         solver_parameters.method = dump[1];
345                     }
346
347                     // Get Parallel
348                     else if (line.rfind("parallel", 0) != std::string::npos)
349                     {
350                         while (std::getline(string_stream, tmp, '='))
351                         {
352                             dump.push_back(tmp);
353                         }
354                         if (dump.size() != 2)
355                         {
356                             std::cerr << "Unexpected Configuration File" << std::endl;
357                         }
358
359                         if (dump[1].rfind("true", 0) != std::string::npos)
360                         {
361                             solver_parameters.run_parallel = true;
362                             filled_parallel = true;
363                         }
364                         else if (dump[1].rfind("false", 0) != std::string::npos)
365                         {
366                             solver_parameters.run_parallel = false;
367                             filled_parallel = true;
368                         }
369                         else{
370                             std::cerr << "Unexpected Configuration File" << std::endl;
371                         }
372                     }
373
374                     // Get Print Info
375                     else if (line.rfind("print_info", 0) != std::string::npos)
376                     {
377                         while (std::getline(string_stream, tmp, '='))
378                         {
379                             dump.push_back(tmp);
380                         }
381                         if (dump.size() != 2)
382                         {
383                             std::cerr << "Unexpected Configuration File" << std::endl;
384                         }
385                         if (dump[1].rfind("true", 0) != std::string::npos)
386                         {
387                             solver_parameters.print_info = true;
388                         }
389                         else if (dump[1].rfind("false", 0) != std::string::npos)
390                         {
391                             solver_parameters.print_info = false;
392                         }
393                         else
394                         {
395                             std::cerr << "Unexpected Configuration File" << std::endl;
396                         }
397                     }
398
399                     // Get Save Data
400                     else if (line.rfind("save_data", 0) != std::string::npos)
401                     {
402                         while (std::getline(string_stream, tmp, '='))
403                         {
404                             dump.push_back(tmp);
405                         }
406                         if (dump.size() != 2)
407                         {
408                             std::cerr << "Unexpected Configuration File" << std::endl;
409                         }
410                         if (dump[1].rfind("true", 0) != std::string::npos)
411                         {
412                             solver_parameters.save_data = true;
413                         }
414                         else if (dump[1].rfind("false", 0) != std::string::npos)
415                         {
416                             solver_parameters.save_data = false;
417                         }
418                         else
```

```
419                         {
420                             std::cerr « "Unexpected Configuration File" « std::endl;
421                         }
422                     }
423 
424                     // Get Cuda Device
425                     else if (line.rfind("cuda_device", 0) != std::string::npos)
426                     {
427                         while (std::getline(string_stream, tmp, '='))
428                         {
429                             dump.push_back(tmp);
430                         }
431                         if (dump.size() != 2)
432                         {
433                             std::cerr « "Unexpected Configuration File" « std::endl;
434                         }
435                         solver_parameters.int_parameters[dump[0]] = std::atoi(dump[1].c_str());
436                     }
437 
438                     // Get max iter
439                     else if (line.rfind("max_iter", 0) != std::string::npos)
440                     {
441                         while (std::getline(string_stream, tmp, '='))
442                         {
443                             dump.push_back(tmp);
444                         }
445                         if (dump.size() != 2)
446                         {
447                             std::cerr « "Unexpected Configuration File" « std::endl;
448                         }
449                         solver_parameters.int_parameters[dump[0]] = std::atoi(dump[1].c_str());
450                     }
451 
452                     else
453                     {
454                         while (std::getline(string_stream, tmp, '='))
455                         {
456                             dump.push_back(tmp);
457                         }
458                         if (dump.size() != 2)
459                         {
460                             std::cerr « "Unexpected Configuration File" « std::endl;
461                         }
462                         if ( (solver_parameters.method != "") && filled_parallel)
463                         {
464                             solver_parameters.solver_parameters[dump[0]] = std::atof(dump[1].c_str());
465                         }
466                         else
467                         {
468                             std::cerr « "Unexpected Configuration File" « std::endl;
469                         }
470                     }
471 
472                 }
473                 else{
474                     std::cerr « "Unexpected Configuration File" « std::endl;
475                 }
476             }
477         }
478     }
479     // setup parameters
480     parameters.main_parameters = main_parameters;
481     parameters.domain_parameters = domain_parameters;
482     parameters.init_cond_parameters = init_parameters;
483     parameters.equation_parameters = equation_parameters;
484     parameters.solver_parameters = solver_parameters;
485     return parameters;
486 }
```

Here is the caller graph for this function:



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

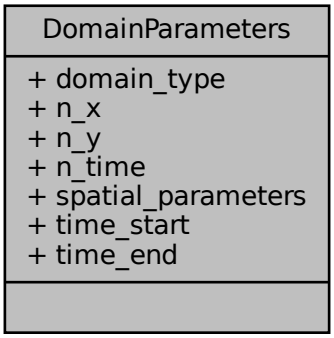
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/config_parser.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/config_parser.cpp

4.8 DomainParameters Class Reference

Domain branch parameters containing information about domain.

`#include <parameters.h>`

Collaboration diagram for DomainParameters:



Public Attributes

- std::string domain_type = std::string("")
- int n_x
- int n_y
- int n_time
- std::map< std::string, float > spatial_parameters
- float time_start
- float time_end

4.8.1 Detailed Description

Domain branch parameters containing information about domain.

Definition at line 33 of file parameters.h.

4.8.2 Member Data Documentation

4.8.2.1 domain_type

```
std::string DomainParameters::domain_type = std::string("")
```

Definition at line 36 of file parameters.h.

4.8.2.2 n_time

```
int DomainParameters::n_time
```

Definition at line 37 of file parameters.h.

4.8.2.3 n_x

```
int DomainParameters::n_x
```

Definition at line 37 of file parameters.h.

4.8.2.4 n_y

```
int DomainParameters::n_y
```

Definition at line 37 of file parameters.h.

4.8.2.5 spatial_parameters

```
std::map<std::string, float> DomainParameters::spatial_parameters
```

Definition at line 38 of file parameters.h.

4.8.2.6 time_end

```
float DomainParameters::time_end
```

Definition at line 39 of file parameters.h.

4.8.2.7 time_start

```
float DomainParameters::time_start
```

Definition at line 39 of file parameters.h.

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

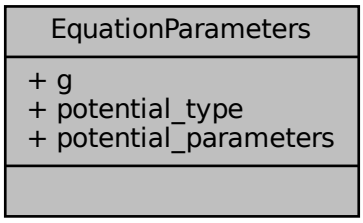
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/parameters.h

4.9 EquationParameters Class Reference

Equation branch parameters containing information about equation.

```
#include <parameters.h>
```

Collaboration diagram for EquationParameters:



Public Attributes

- float g
- std::string potential_type = std::string("")
- std::map< std::string, float > potential_parameters

4.9.1 Detailed Description

Equation branch parameters containing information about equation.

Definition at line 57 of file parameters.h.

4.9.2 Member Data Documentation

4.9.2.1 g

```
float EquationParameters::g
```

Definition at line 60 of file parameters.h.

4.9.2.2 potential_parameters

```
std::map<std::string, float> EquationParameters::potential_parameters
```

Definition at line 62 of file parameters.h.

4.9.2.3 potential_type

```
std::string EquationParameters::potential_type = std::string("")
```

Definition at line 61 of file parameters.h.

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

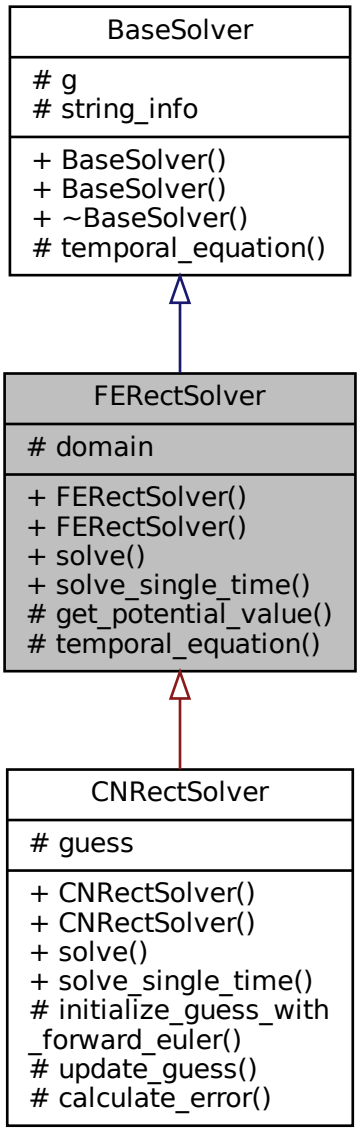
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/parameters.h

4.10 FERectSolver Class Reference

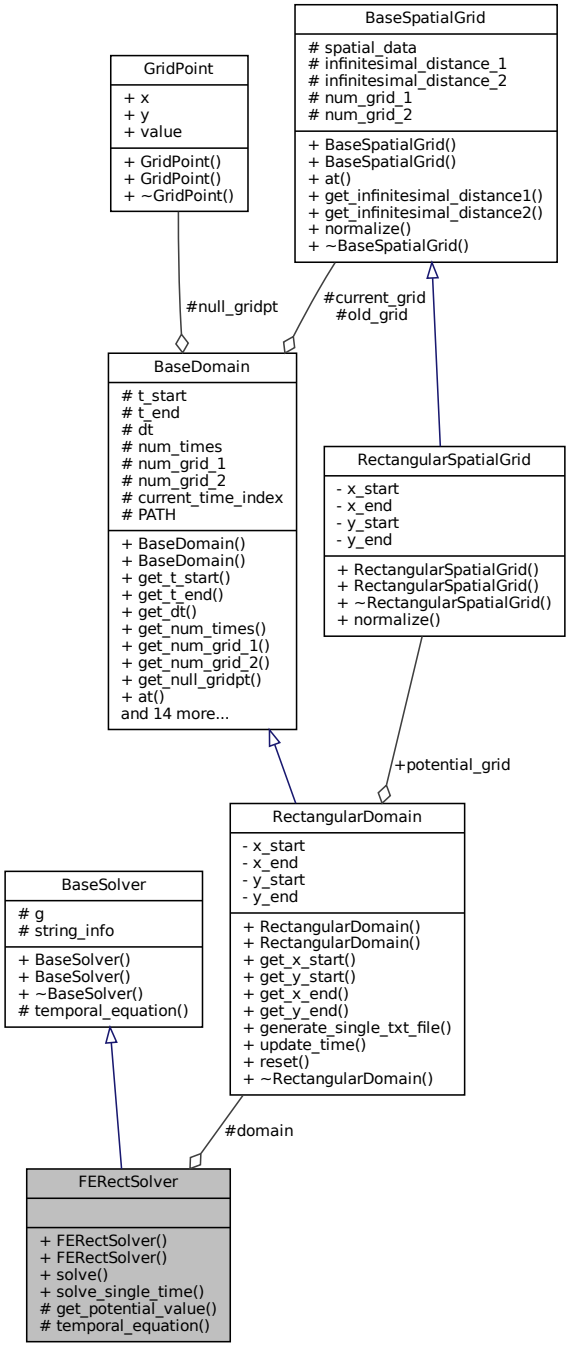
Forward Euler Serial Solver.

```
#include <fe_rect_solver.h>
```

Inheritance diagram for FERectSolver:



Collaboration diagram for FERectSolver:



Public Member Functions

- FERectSolver ()=default
- FERectSolver (float g, RectangularDomain *domain)

  Construct a new FERectSolver::FERectSolver object.
- void solve (std::string dir_name="", bool print_info=true, bool save_data=true)

  Solve Equation.

- void solve_single_time (int k)

  Update k+1 th wave function value with k th values.

Protected Member Functions

- float get_potential_value (int i, int j)

  Get Potential value on each grid point.
- std::complex< float > temporal_equation (int i, int j, int k)

  Time differential of phi.

Protected Attributes

- RectangularDomain * domain
- float g
- std::string string_info

4.10.1 Detailed Description

Forward Euler Serial Solver.

Definition at line 27 of file fe_rect_solver.h.

4.10.2 Constructor & Destructor Documentation

4.10.2.1 FERectSolver() [1/2]

```
FERectSolver::FERectSolver ( )  [default]
```

4.10.2.2 FERectSolver() [2/2]

```
FERectSolver::FERectSolver (
            float g_,
            RectangularDomain * domain_ )
```

Construct a new FERectSolver::FERectSolver object.

Parameters

*g_*	
*domain_*	

Definition at line 20 of file fe_rect_solver.cpp.

```
23     : BaseSolver(g_)
24 {
25     this->domain = domain_;
26     this->string_info = std::string{"Forward_Euler_serial_"};
27
28 };
```

4.10.3 Member Function Documentation

4.10.3.1 get_potential_value()

```
float FERectSolver::get_potential_value (
            int i,
            int j )  [protected]
```

Get Potential value on each grid point.

Parameters

i	
j	

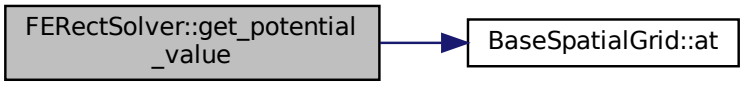
Returns

float

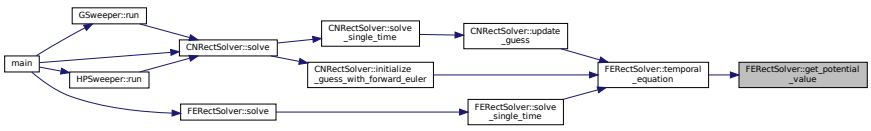
Definition at line 37 of file fe_rect_solver.cpp.

```
38 {
39
40     return this->domain->potential_grid->at(i, j)->value.real();
41 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.10.3.2 solve()

```
void FERectSolver::solve (
            std::string dir_name = "",
            bool print_info = true,
            bool save_data = true )
```

Solve Equation.

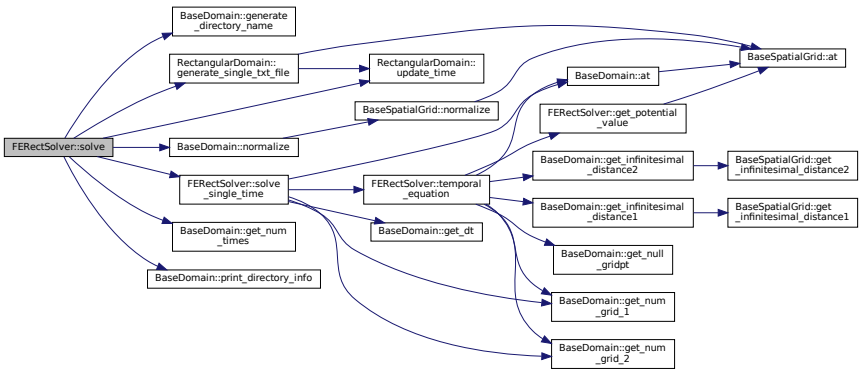
Parameters

dir_name	
print_info	
save_data	

Definition at line 116 of file fe_rect_solver.cpp.

```
117 {
118     int time_length = this->domain->get_num_times();
119     if(save_data){
120         this->domain->generate_directory_name(this->string_info+dir_name, print_info);
121         //Save initial condition
122         this->domain->generate_single_txt_file(std::string("Solution_") + std::to_string(0));
123     }else{
124         this -> domain->update_time();
125     }
126
127     for (int k = 0; k < time_length - 1; ++k)
128     {
129         this->solve_single_time(k);
130         this->domain->normalize(k + 1);
131         if(save_data){
132             this->domain->generate_single_txt_file(std::string("Solution_") + std::to_string(k + 1));
133         }
134         else{
135             this->domain->update_time();
136         }
137     }
138     if(print_info){
139         this->domain->print_directory_info();
140     }
141 }
```

Here is the call graph for this function:



Here is the caller graph for this function:

4.10.3.3 solve_single_time()

```
void FERectSolver::solve_single_time (
            int k )
```

Update k+1 th wave function value with k th values.

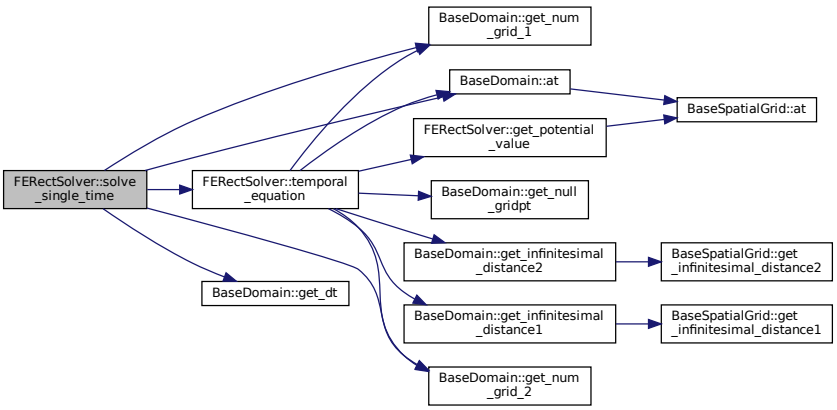
Parameters

k	

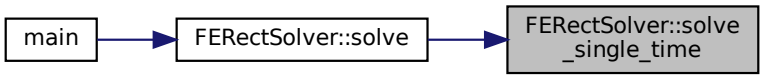
Definition at line 95 of file fe_rect_solver.cpp.

```
96 {
97     int Nx = this->domain->get_num_grid_1();
98     int Ny = this->domain->get_num_grid_2();
99     float dt = this->domain->get_dt();
100     for (int i = 0; i < Nx; ++i)
101     {
102         for (int j = 0; j < Ny; ++j)
103         {
104             (this->domain->at(i, j, k + 1)->value) = this->domain->at(i, j, k)->value + dt *
       this->temporal_equation(i, j, k);
105         }
106     }
107 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.10.3.4 temporal_equation()

```
std::complex< float > FERectSolver::temporal_equation (
            int i,
            int j,
            int k )  [protected]
```

Time differential of phi.

Parameters

i	index for x
j	index for y
k	index for time(t)

Returns

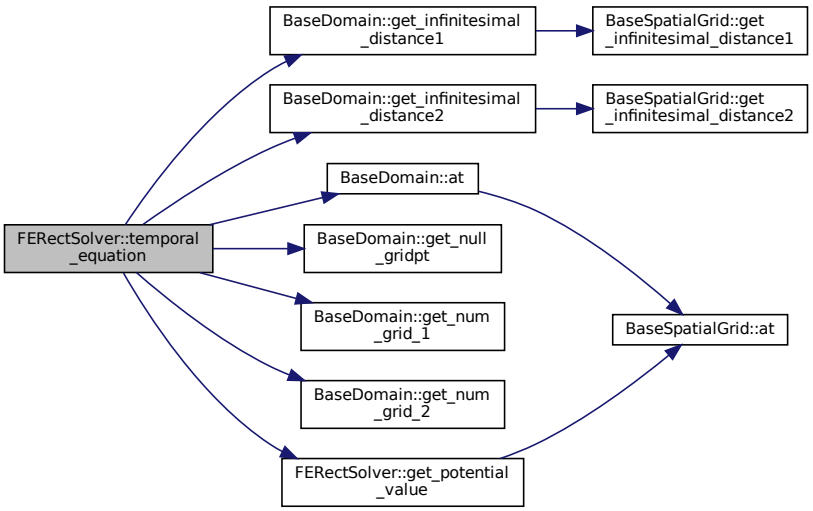
std::complex<float> time differential at x, y, t

Definition at line 51 of file fe_rect_solver.cpp.

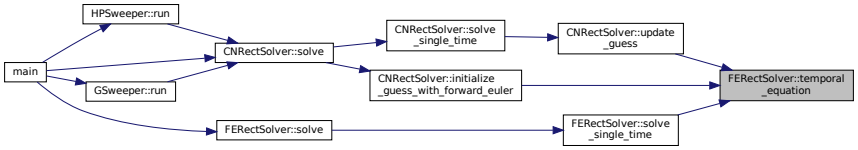
```
52 {
53     //Use five stencil method
54     auto point_data = this->domain->at(i, j, k);
55 
56     //l,r,d,u denotes left, right, down, up value
57     //Check boundary
58     auto point_data_l = this->domain->at(i - 1, j, k);
59     if (i <= 0)
60         point_data_l = this->domain->get_null_gridpt();
61     auto point_data_d = this->domain->at(i, j - 1, k);
62     if (j <= 0)
63         point_data_d = this->domain->get_null_gridpt();
64     auto point_data_r = this->domain->at(i + 1, j, k);
65     if (i >= (this->domain->get_num_grid_1()) - 1)
66         point_data_r = this->domain->get_null_gridpt();
67     auto point_data_u = this->domain->at(i, j + 1, k);
68     if (j >= (this->domain->get_num_grid_2()) - 1)
69         point_data_u = this->domain->get_null_gridpt();
70 
71     //potential at x, y
72     float V_ij = this->get_potential_value(i, j);
73     //this->potential_func(point_data->x, point_data->y);
74 
75     //g * |psi(x,y)|^2
76     float additional_term = (this->g) * (std::abs(point_data->value)) * (std::abs(point_data->value));
77 
78     //Set infinitesimal value
79     float dx = this->domain->get_infinitesimal_distance1();
80     float dy = this->domain->get_infinitesimal_distance2();
```

```
81     //df denote time differential of dt (d(psi)/dt)
82     // = (laplace - V-g|psi|^2) psi
83     std::complex<float> df =
84         +((point_data_r->value) + (point_data_l->value) - (point_data->value) * std::complex<float>{2}) /
       (std::complex<float>{dx * dx}) + ((point_data_u->value) + (point_data_d->value) - (point_data->value)
       * std::complex<float>{2}) / (std::complex<float>{dy * dy}) - (V_ij + additional_term) *
       (point_data->value);
85     df *= std::complex<float>{0, 1};
86
87     return df;
88 };
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.10.4 Member Data Documentation

4.10.4.1 domain

```
RectangularDomain* FERectSolver::domain  [protected]
```

Definition at line 39 of file fe_rect_solver.h.

4.10.4.2 g

```
float BaseSolver::g  [protected], [inherited]
```

Definition at line 30 of file base_solver.h.

4.10.4.3 string_info

```
std::string BaseSolver::string_info  [protected], [inherited]
```

Definition at line 32 of file base_solver.h.

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

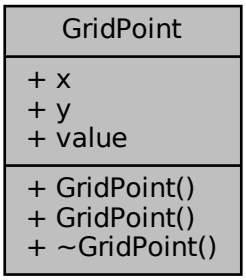
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/solver/serial_solver/forward_euler/fe_rect_solver.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/solver/serial_solver/forward_euler/fe_rect_solver.cpp

4.11 GridPoint Class Reference

Grid point class (single point)

```
#include <base_domain.h>
```

Collaboration diagram for GridPoint:



Public Member Functions

- GridPoint ()=default
- GridPoint (float x, float y, std::complex< float > wave_function)
- ~GridPoint ()

Public Attributes

- float x
- float y
- std::complex< float > value

4.11.1 Detailed Description

Grid point class (single point)

Definition at line 31 of file base_domain.h.

4.11.2 Constructor & Destructor Documentation

4.11.2.1 GridPoint() [1/2]

```
GridPoint::GridPoint ( )  [default]
```

4.11.2.2 GridPoint() [2/2]

```
GridPoint::GridPoint (
            float x,
            float y,
            std::complex< float > wave_function )
```

Definition at line 13 of file base_domain.cpp.

```
13 : x(x_), y(y_), value(wave_function_) {}
```

4.11.2.3 ~GridPoint()

```
GridPoint::~GridPoint ( )
```

Definition at line 14 of file base_domain.cpp.

```
14 {};
```

4.11.3 Member Data Documentation

4.11.3.1 value

```
std::complex<float> GridPoint::value
```

Definition at line 38 of file base_domain.h.

4.11.3.2 x

```
float GridPoint::x
```

Definition at line 36 of file base_domain.h.

4.11.3.3 y

```
float GridPoint::y
```

Definition at line 36 of file base_domain.h.

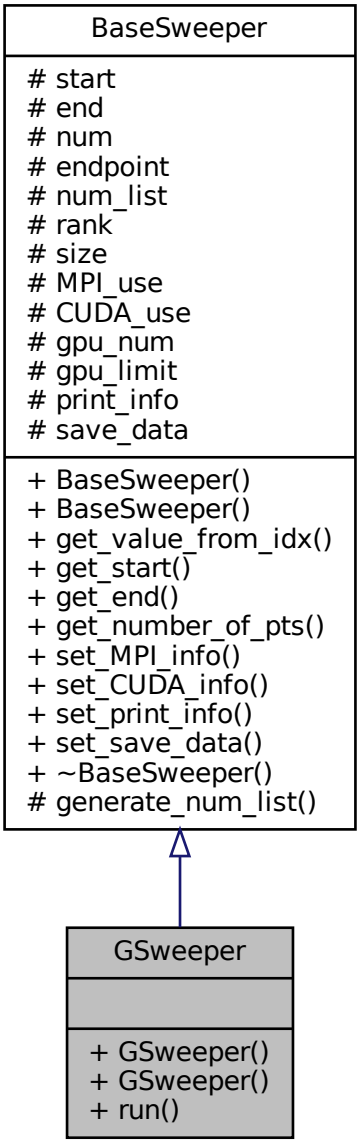
The documentation for this class was generated from the following files:

- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/domain/base_domain.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/domain/base_domain.cpp

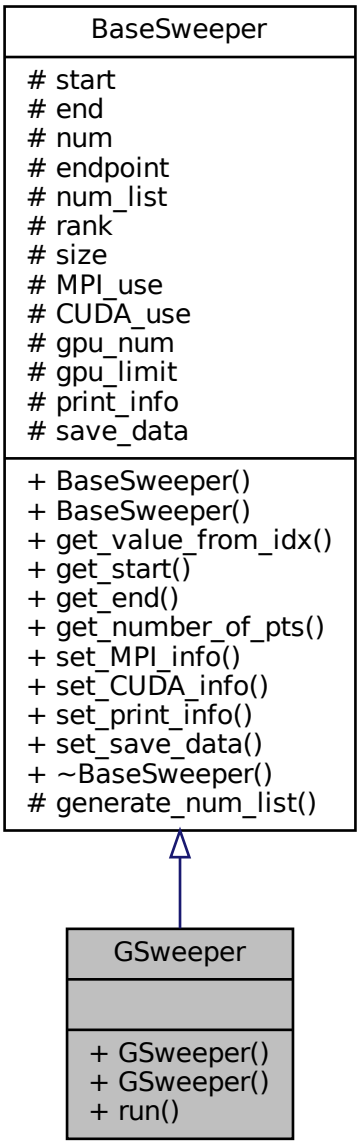
4.12 GSweeper Class Reference

```
#include <g_sweeper.h>
```

Inheritance diagram for GSweeper:



Collaboration diagram for GSweeper:



Public Member Functions

- GSweeper ()=default
- GSweeper (float start, float end, int num, bool endpoint)
- void run (RectangularDomain *domain, InitialCondition *initial_condition, HarmonicPotential *potential)
- float get_value_from_idx (int idx)
- float get_start ()
- float get_end ()
- int get_number_of_pts ()
- virtual void set_MPI_info (int rank, int size)

- virtual void set_CUDA_info (int gpu_num, int gpu_limit)
- void set_print_info (bool print_info)
- void set_save_data (bool save_data)

Protected Member Functions

- void generate_num_list ()

  generate number of points that sweep from start to end

Protected Attributes

- float start
- float end
- int num
- bool endpoint
- vector< float > num_list
- int rank =0
- int size =0
- bool MPI_use
- bool CUDA_use
- int gpu_num =1
- int gpu_limit =3
- bool print_info =true
- bool save_data =true

4.12.1 Detailed Description

Definition at line 5 of file g_sweeper.h.

4.12.2 Constructor & Destructor Documentation

4.12.2.1 GSweeper() [1/2]

```
GSweeper::GSweeper ( )  [default]
```

4.12.2.2 GSweeper() [2/2]

```
GSweeper::GSweeper (
            float start,
            float end,
            int num,
            bool endpoint )
```

Definition at line 7 of file g_sweeper.cpp.

```
8 : BaseSweeper(start, end, num, endpoint){
9
10 }
```

4.12.3 Member Function Documentation

4.12.3.1 generate_num_list()

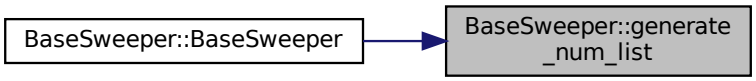
```
void BaseSweeper::generate_num_list ( )  [protected], [inherited]
```

generate number of points that sweep from start to end

Definition at line 15 of file base_sweeper.cpp.

```
15                                      {
16     this->num_list = std::vector<float>(this->num);
17     float d = 0.;
18     if(this->endpoint){
19         d = (this -> end - this-> start ) / float(this-> num -1 );
20     }else{
21         d = (this -> end - this-> start ) / float(this-> num);
22     }
23
24     for (int i=0; i<this -> num; ++i){
25         this->num_list[i] = this ->start + d*i;
26     }
27
28 }
```

Here is the caller graph for this function:



4.12.3.2 get_end()

```
float BaseSweeper::get_end ( )  [inherited]
```

Definition at line 38 of file base_sweeper.cpp.

```
38                              {
39     return end;
40 }
```

4.12.3.3 get_number_of_pts()

```
int BaseSweeper::get_number_of_pts ( )  [inherited]
```

Definition at line 41 of file base_sweeper.cpp.

```
41                                      {
42     return num;
43 }
```

4.12.3.4 get_start()

```
float BaseSweeper::get_start ( )  [inherited]
```

Definition at line 35 of file base_sweeper.cpp.

```
35                              {
36     return start;
37 }
```

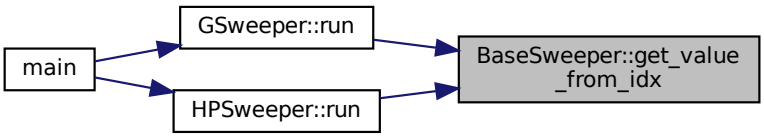
4.12.3.5 get_value_from_idx()

```
float BaseSweeper::get_value_from_idx (
              int idx )  [inherited]
```

Definition at line 31 of file base_sweeper.cpp.

```
31                                          {
32     return this->num_list[idx];
33 }
```

Here is the caller graph for this function:



4.12.3.6 run()

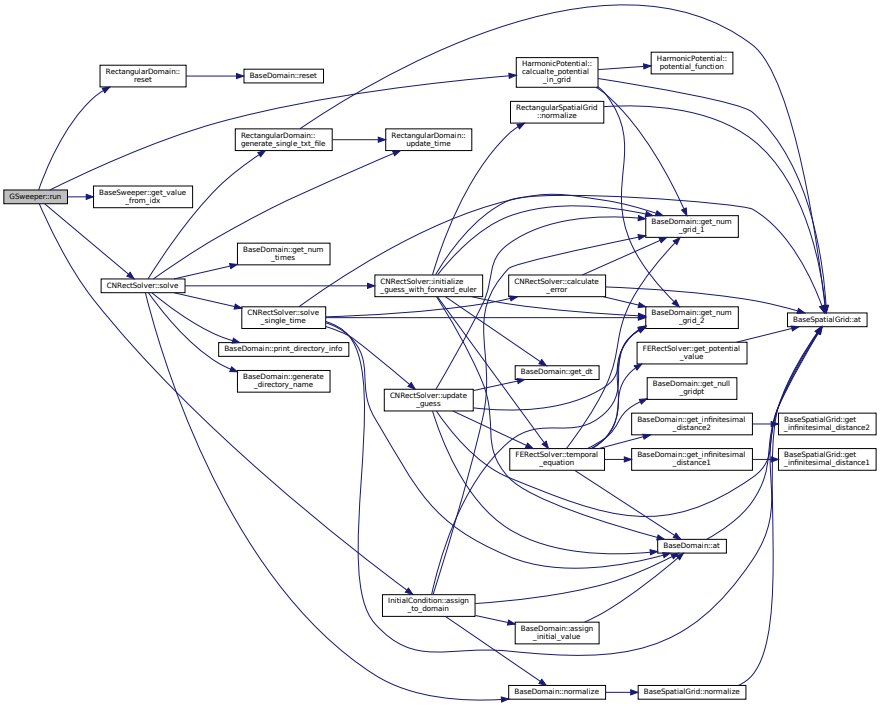
```
void GSweeper::run (
              RectangularDomain * domain,
              InitialCondition * initial_condition,
              HarmonicPotential * potential )
```

Definition at line 12 of file g_sweeper.cpp.

```
12
            {
13
14
15     if (!(this -> MPI_use) && !(this -> CUDA_use)){
16         if(print_info){
17             cout« "Running serially started"«endl;
18         }
19         float g=0;
20         for(int i=0; i<this -> num ; ++i){
21             //Set conditions
22             initial_condition->assign_to_domain(domain);
23             potential->calcualte_potential_in_grid(domain);
24             g = this  -> get_value_from_idx(i);
25             //Apply on solver
26             CNRectSolver* solver =new CNRectSolver(g, domain);
27             //solve using solver. It automatically save data
```

```
28              solver->solve(1e-11, 101, to_string(i) , this-> print_info, this -> save_data);
29              //reset domain to use in next iteration
30              domain->reset();
31              delete solver;
32          }
33      }
34      else if ((this->MPI_use) && !(this->CUDA_use)){
35          //If number of tasks exceed number of processors, abort.
36          if(print_info){
37              cout« "Running with only MPI started"«endl;
38          }
39          if (num > size){
40              MPI_Abort( MPI_COMM_WORLD, EXIT_FAILURE);
41          }
42          float g = 0 ;
43          if (rank < num){
44              initial_condition->assign_to_domain(domain);
45              potential->calcualte_potential_in_grid(domain);
46              g = this  -> get_value_from_idx(rank);
47              CNRectSolver* solver =new CNRectSolver(g, domain);
48              solver->solve(1e-11, 101, "MPI_"+to_string(rank), this -> print_info, this->save_data);
49              delete solver;
50          }else{
51              // No job for extra processors
52              ;
53          }
54      }else if (!(this->MPI_use) && (this->CUDA_use)){
55
56          if(print_info){
57              cout« "Running with CUDA serially started"«endl;
58          }
59          float g=0;
60          for(int i=0; i<this -> num ; ++i){
61              //Set conditions
62              initial_condition->assign_to_domain(domain);
63              potential->calcualte_potential_in_grid(domain);
64              g = this  -> get_value_from_idx(i);
65              //Apply on solver
66              CNRectPSolver* solver =new CNRectPSolver(g, domain, 0);//solve using solver. It automatically
    save data
67              solver->solve(1e-11, 101, "CUDA_"+to_string(i) , this-> print_info, this -> save_data);
68              //reset domain to use in next iteration
69              domain->reset();
70              delete solver;
71          }
72
73      }
74      else{
75          if(print_info){
76              cout« "Running with CUDA & MPI started"«endl;
77          }
78          float g=0;
79
80          if (num > size){
81              MPI_Abort( MPI_COMM_WORLD, EXIT_FAILURE);
82          }
83          int max_pallel_tasks = this -> gpu_num * this ->gpu_limit;
84          int repeat = num / max_pallel_tasks+(num%max_pallel_tasks !=0);
85          for(int i=0; i<repeat; ++i){
86              if (i*repeat < max_pallel_tasks && rank < (i+1)*max_pallel_tasks && rank < num ){
87                  int casted_GPU_num = (rank % max_pallel_tasks) % gpu_limit;
88                  initial_condition->assign_to_domain(domain);
89                  potential->calcualte_potential_in_grid(domain);
90                  g = this  -> get_value_from_idx(rank);
91                  CNRectPSolver* solver =new CNRectPSolver(g, domain, casted_GPU_num);
92                  solver->solve(1e-11, 101, "MPI&CUDA_"+to_string(rank), this -> print_info,
    this->save_data);
93                  delete solver;
94              }
95          }
96
97
98
99      }
100 }
```

Here is the call graph for this function:



Here is the caller graph for this function:

4.12.3.7 set_CUDA_info()

```
void BaseSweeper::set_CUDA_info (
            int gpu_num,
            int gpu_limit )  [virtual], [inherited]
```

Definition at line 51 of file base_sweeper.cpp.

```
51                                                  {
52     this -> CUDA_use=true;
53     this -> gpu_num = gpu_num;
54     this -> gpu_limit = gpu_limit;
55 }
```

Here is the caller graph for this function:

4.12.3.8 set_MPI_info()

```
void BaseSweeper::set_MPI_info (
            int rank,
            int size )  [virtual], [inherited]
```

Definition at line 45 of file base_sweeper.cpp.

```
45                                                {
46     this -> rank = rank;
47     this -> size = size;
48     this -> MPI_use=true;
49 }
```

Here is the caller graph for this function:

4.12.3.9 set_print_info()

```
void BaseSweeper::set_print_info (
            bool print_info )  [inherited]
```

Definition at line 57 of file base_sweeper.cpp.

```
57                                                {
58     this -> print_info = print_info;
59 }
```

Here is the caller graph for this function:

4.12.3.10 set_save_data()

```
void BaseSweeper::set_save_data (
            bool save_data )  [inherited]
```

Definition at line 60 of file base_sweeper.cpp.

```
60                                          {
61     this -> save_data = save_data;
62 }
```

Here is the caller graph for this function:

4.12.4 Member Data Documentation

4.12.4.1 CUDA_use

```
bool BaseSweeper::CUDA_use  [protected], [inherited]
```

Definition at line 36 of file base_sweeper.h.

4.12.4.2 end

```
float BaseSweeper::end  [protected], [inherited]
```

Definition at line 25 of file base_sweeper.h.

4.12.4.3 endpoint

```
bool BaseSweeper::endpoint  [protected], [inherited]
```

Definition at line 27 of file base_sweeper.h.

4.12.4.4 gpu_limit

```
int BaseSweeper::gpu_limit =3  [protected], [inherited]
```

Definition at line 38 of file base_sweeper.h.

4.12.4.5 gpu_num

```
int BaseSweeper::gpu_num =1  [protected], [inherited]
```

Definition at line 37 of file base_sweeper.h.

4.12.4.6 MPI_use

```
bool BaseSweeper::MPI_use  [protected], [inherited]
```

Definition at line 34 of file base_sweeper.h.

4.12.4.7 num

```
int BaseSweeper::num  [protected], [inherited]
```

Definition at line 26 of file base_sweeper.h.

4.12.4.8 num_list

```
vector<float> BaseSweeper::num_list  [protected], [inherited]
```

Definition at line 28 of file base_sweeper.h.

4.12.4.9 print_info

```
bool BaseSweeper::print_info =true  [protected], [inherited]
```

Definition at line 40 of file base_sweeper.h.

4.12.4.10 rank

```
int BaseSweeper::rank =0  [protected], [inherited]
```

Definition at line 32 of file base_sweeper.h.

4.12.4.11 save_data

```
bool BaseSweeper::save_data =true  [protected], [inherited]
```

Definition at line 41 of file base_sweeper.h.

4.12.4.12 size

```
int BaseSweeper::size =0  [protected], [inherited]
```

Definition at line 33 of file base_sweeper.h.

4.12.4.13 start

```
float BaseSweeper::start  [protected], [inherited]
```

Definition at line 24 of file base_sweeper.h.

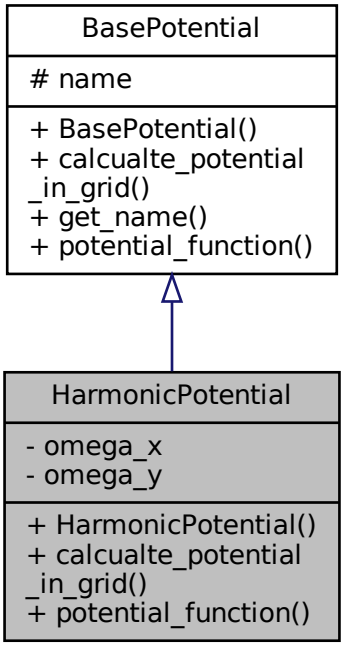
The documentation for this class was generated from the following files:

- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/sweeper/g_sweeper.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/sweeper/g_sweeper.cpp

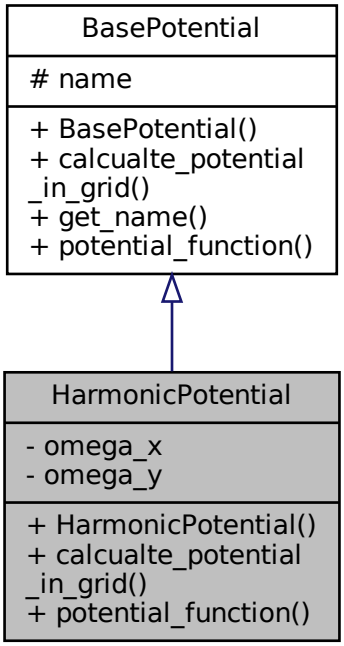
4.13 HarmonicPotential Class Reference

`#include <harmonic_potential.h>`

Inheritance diagram for HarmonicPotential:



Collaboration diagram for HarmonicPotential:



Public Member Functions

- HarmonicPotential (float omega_x, float omega_y)

  Construct a new Harmonic Potential:: Harmonic Potential object V = 0.5 ∗ (omega_x^2 ∗ x^2 + omega_y^2 ∗ y^2)
- void calcualte_potential_in_grid (RectangularDomain ∗domain)
- float potential_function (float x, float y)
- std::string get_name ()

  Getter for name class variable.

Protected Attributes

- std::string name

Private Attributes

- float omega_x
- float omega_y

4.13.1 Detailed Description

Definition at line 19 of file harmonic_potential.h.

4.13.2 Constructor & Destructor Documentation

4.13.2.1 HarmonicPotential()

```
HarmonicPotential::HarmonicPotential (
            float omega_x,
            float omega_y )
```

Construct a new Harmonic Potential:: Harmonic Potential object V = 0.5 ∗ (omega_x^2 ∗ x^2 + omega_y^2 ∗ y^2)

Parameters

omega_x	
omega_y	

Definition at line 19 of file harmonic_potential.cpp.

```
20 : BasePotential(), omega_x(omega_x), omega_y(omega_y)
21 {
22     this->name = std::string("Harmonic");
23 }
```

4.13.3 Member Function Documentation

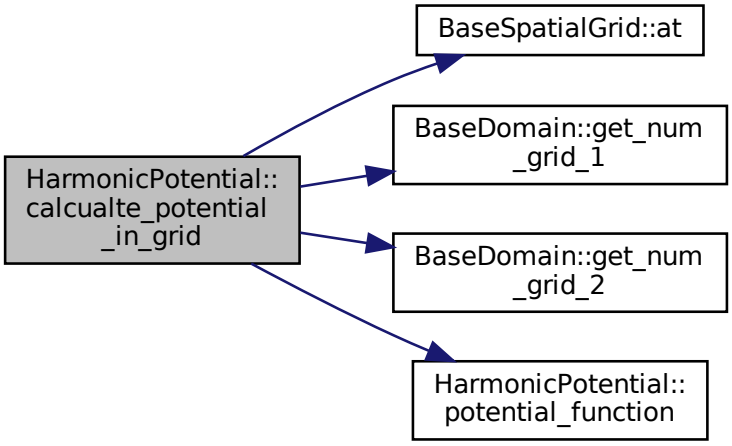
4.13.3.1 calcualte_potential_in_grid()

```
void HarmonicPotential::calcualte_potential_in_grid (
            RectangularDomain * domain )
```

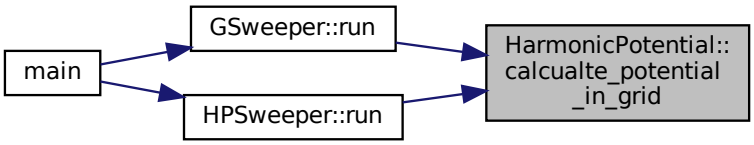
Definition at line 29 of file harmonic_potential.cpp.

```
30 {
31     int num_grid_1 = domain->get_num_grid_1();
32     int num_grid_2 = domain->get_num_grid_2();
33     for (auto i = 0; i < num_grid_1; ++i)
34     {
35         for (auto j = 0; j < num_grid_2; ++j)
36         {
37             auto point = domain->potential_grid->at(i, j);
38
39             //Assign potential value in potential grid
40             point->value = std::complex<float>{this->potential_function(point->x, point->y), 0};
41         }
42     }
43 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.13.3.2 get_name()

```
std::string BasePotential::get_name ( )  [inherited]
```

Getter for name class variable.

Returns

std::string

Definition at line 40 of file base_potential.cpp.

```
41 {
42     return this->name;
43 }
```

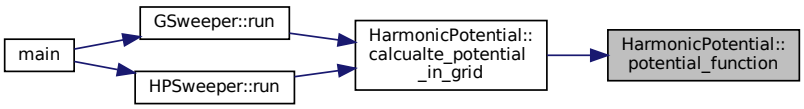
4.13.3.3 potential_function()

```
float HarmonicPotential::potential_function (
            float x,
            float y )
```

Definition at line 25 of file harmonic_potential.cpp.

```
26 {
27     return 0.5 * (this->omega_x * x * x + this->omega_y * y * y);
28 }
```

Here is the caller graph for this function:



4.13.4 Member Data Documentation

4.13.4.1 name

```
std::string BasePotential::name  [protected], [inherited]
```

Definition at line 27 of file base_potential.h.

4.13.4.2 omega_x

```
float HarmonicPotential::omega_x  [private]
```

Definition at line 27 of file harmonic_potential.h.

4.13.4.3 omega_y

```
float HarmonicPotential::omega_y  [private]
```

Definition at line 27 of file harmonic_potential.h.

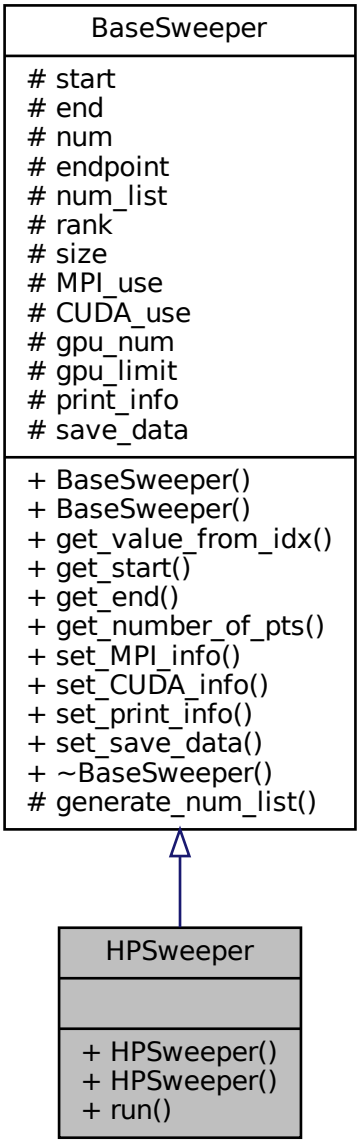
The documentation for this class was generated from the following files:

- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/potential/harmonic_potential.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/potential/harmonic_potential.cpp

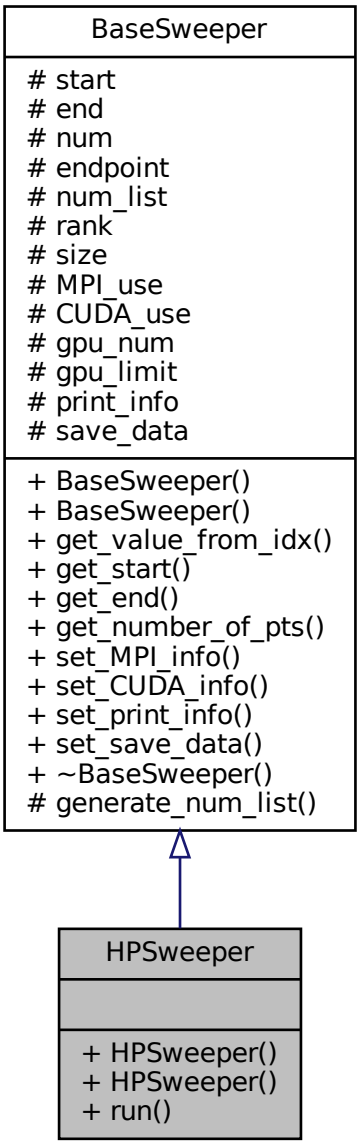
4.14 HPSweeper Class Reference

```
#include <harmonic_p_sweeper.h>
```

Inheritance diagram for HPSweeper:



Collaboration diagram for HPSweeper:



Public Member Functions

- HPSweeper ()=default
- HPSweeper (float start, float end, int num, bool endpoint)
- void run (RectangularDomain *domain, InitialCondition *initial_condition, float g)
- float get_value_from_idx (int idx)
- float get_start ()
- float get_end ()
- int get_number_of_pts ()
- virtual void set_MPI_info (int rank, int size)

- virtual void set_CUDA_info (int gpu_num, int gpu_limit)
- void set_print_info (bool print_info)
- void set_save_data (bool save_data)

Protected Member Functions

- void generate_num_list ()

  generate number of points that sweep from start to end

Protected Attributes

- float start
- float end
- int num
- bool endpoint
- vector< float > num_list
- int rank =0
- int size =0
- bool MPI_use
- bool CUDA_use
- int gpu_num =1
- int gpu_limit =3
- bool print_info =true
- bool save_data =true

4.14.1 Detailed Description

Definition at line 5 of file harmonic_p_sweeper.h.

4.14.2 Constructor & Destructor Documentation

4.14.2.1 HPSweeper() [1/2]

```
HPSweeper::HPSweeper ( )  [default]
```

4.14.2.2 HPSweeper() [2/2]

```
HPSweeper::HPSweeper (
            float start,
            float end,
            int num,
            bool endpoint )
```

Definition at line 7 of file harmonic_p_sweeper.cpp.

```
8 : BaseSweeper(start, end, num, endpoint){
9     //numlist contains assymetry of angular frequency
10 }
```

4.14.3 Member Function Documentation

4.14.3.1 generate_num_list()

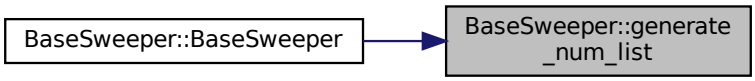
```
void BaseSweeper::generate_num_list ( )  [protected], [inherited]
```

generate number of points that sweep from start to end

Definition at line 15 of file base_sweeper.cpp.

```
15                                      {
16     this->num_list = std::vector<float>(this->num);
17     float d = 0.;
18     if(this->endpoint){
19         d = (this -> end - this-> start ) / float(this-> num -1 );
20     }else{
21         d = (this -> end - this-> start ) / float(this-> num);
22     }
23
24     for (int i=0; i<this -> num; ++i){
25         this->num_list[i] = this ->start + d*i;
26     }
27
28 }
```

Here is the caller graph for this function:



4.14.3.2 get_end()

```
float BaseSweeper::get_end ( )  [inherited]
```

Definition at line 38 of file base_sweeper.cpp.

```
38                              {
39     return end;
40 }
```

4.14.3.3 get_number_of_pts()

```
int BaseSweeper::get_number_of_pts ( )  [inherited]
```

Definition at line 41 of file base_sweeper.cpp.

```
41                                      {
42     return num;
43 }
```

4.14.3.4 get_start()

```
float BaseSweeper::get_start ( )  [inherited]
```

Definition at line 35 of file base_sweeper.cpp.

```
35                              {
36     return start;
37 }
```

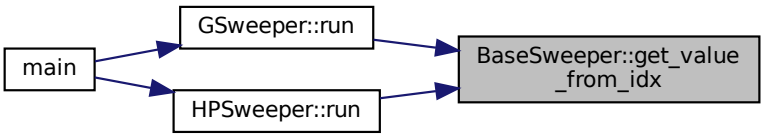
4.14.3.5 get_value_from_idx()

```
float BaseSweeper::get_value_from_idx (
            int idx )  [inherited]
```

Definition at line 31 of file base_sweeper.cpp.

```
31                                          {
32     return this->num_list[idx];
33 }
```

Here is the caller graph for this function:



4.14.3.6 run()

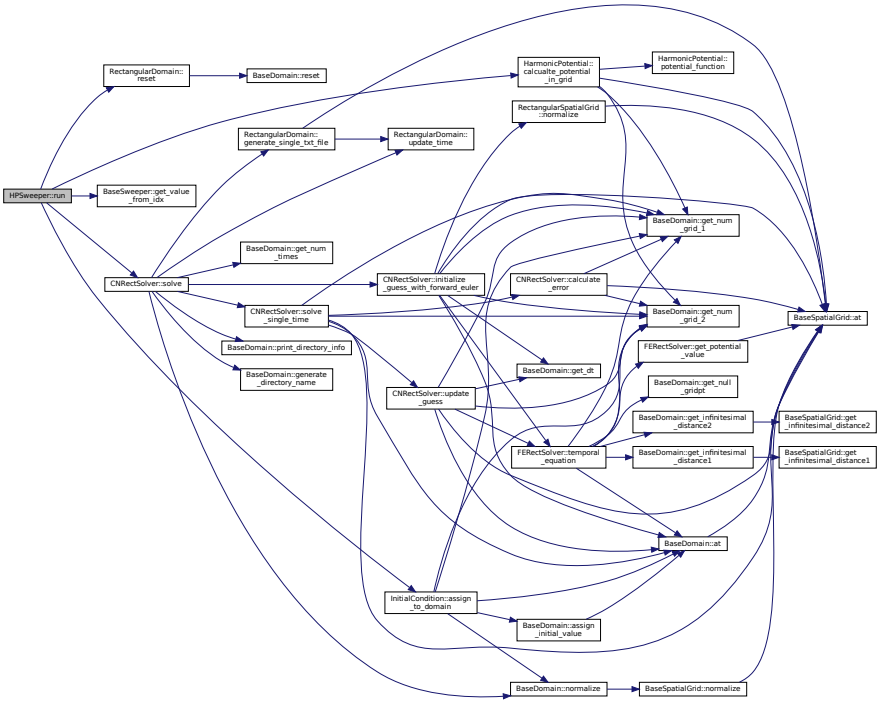
```
void HPSweeper::run (
            RectangularDomain * domain,
            InitialCondition * initial_condition,
            float g )
```

Definition at line 12 of file harmonic_p_sweeper.cpp.

```
12                                                                                                  {
13
14
15     if (!(this -> MPI_use) && !(this -> CUDA_use)){
16         if(print_info){
17             cout« "Running serially started"«endl;
18         }
19
20         for(int i=0; i<this -> num ; ++i){
21             //Set conditions
22             initial_condition->assign_to_domain(domain);
23             HarmonicPotential * potential = new HarmonicPotential(1, get_value_from_idx(i));
24             potential->calcualte_potential_in_grid(domain);
25             g = this  -> get_value_from_idx(i);
26             //Apply on solver
27             CNRectSolver* solver =new CNRectSolver(g, domain);
28             //solve using solver. It automatically save data
```

```
29              solver->solve(1e-11, 101, to_string(i) , this-> print_info, this -> save_data);
30              //reset domain to use in next iteration
31              domain->reset();
32              delete solver;
33              delete potential;
34          }
35      }
36      else if ((this->MPI_use) && !(this->CUDA_use)){
37          //If number of tasks exceed number of processors, abort.
38          if(print_info){
39              cout« "Running with only MPI started"«endl;
40          }
41          if (num > size){
42              MPI_Abort( MPI_COMM_WORLD, EXIT_FAILURE);
43          }
44          float g = 0 ;
45          if (rank < num){
46              initial_condition->assign_to_domain(domain);
47              HarmonicPotential * potential =new HarmonicPotential(1, get_value_from_idx(rank));
48              potential -> calcualte_potential_in_grid(domain);
49              CNRectSolver* solver =new CNRectSolver(g, domain);
50              solver->solve(1e-11, 101, "MPI_"+to_string(rank), this -> print_info, this->save_data);
51              delete solver;
52              delete potential;
53          }else{
54              // No job for extra processors
55              ;
56          }
57      }else if (!(this->MPI_use) && (this->CUDA_use)){
58
59          if(print_info){
60              cout« "Running with CUDA serially started"«endl;
61          }
62          for(int i=0; i<this -> num ; ++i){
63              //Set conditions
64              initial_condition->assign_to_domain(domain);
65              HarmonicPotential * potential = new HarmonicPotential(1, get_value_from_idx(i));
66              potential->calcualte_potential_in_grid(domain);
67              //Apply on solver
68              CNRectPSolver* solver =new CNRectPSolver(g, domain, 0);//solve using solver. It automatically
    save data
69              solver->solve(1e-11, 101, "CUDA_"+to_string(i) , this-> print_info, this -> save_data);
70              //reset domain to use in next iteration
71              domain->reset();
72              delete solver;
73              delete potential;
74          }
75
76      }
77      else{
78          if(print_info){
79              cout« "Running with CUDA & MPI started"«endl;
80          }
81          float g=0;
82
83          if (num > size){
84              MPI_Abort( MPI_COMM_WORLD, EXIT_FAILURE);
85          }
86          int max_pallel_tasks = this -> gpu_num * this ->gpu_limit;
87          int repeat = num / max_pallel_tasks+(num%max_pallel_tasks !=0);
88          for(int i=0; i<repeat; ++i){
89              if (i*repeat < max_pallel_tasks && rank < (i+1)*max_pallel_tasks && rank < num ){
90                  int casted_GPU_num = (rank % max_pallel_tasks) % gpu_limit;
91                  initial_condition->assign_to_domain(domain);
92                  auto potential = new HarmonicPotential(1, get_value_from_idx(rank));
93                  potential->calcualte_potential_in_grid(domain);
94                  //g = this  -> get_value_from_idx(rank);
95                  CNRectPSolver* solver =new CNRectPSolver(g, domain, casted_GPU_num);
96                  solver->solve(1e-11, 101, "MPI&CUDA_"+to_string(rank), this -> print_info,
    this->save_data);
97                  delete solver;
98                  delete potential;
99              }
100         }
101
102
103
104     }
105 }
```

Here is the call graph for this function:



Here is the caller graph for this function:

4.14.3.7 set_CUDA_info()

```
void BaseSweeper::set_CUDA_info (
            int gpu_num,
            int gpu_limit )  [virtual], [inherited]
```

Definition at line 51 of file base_sweeper.cpp.

```
51                                                  {
52     this -> CUDA_use=true;
53     this -> gpu_num = gpu_num;
54     this -> gpu_limit = gpu_limit;
55 }
```

Here is the caller graph for this function:

4.14.3.8 set_MPI_info()

```
void BaseSweeper::set_MPI_info (
            int rank,
            int size )  [virtual], [inherited]
```

Definition at line 45 of file base_sweeper.cpp.

```
45                                                {
46     this -> rank = rank;
47     this -> size = size;
48     this -> MPI_use=true;
49 }
```

Here is the caller graph for this function:

4.14.3.9 set_print_info()

```
void BaseSweeper::set_print_info (
            bool print_info )  [inherited]
```

Definition at line 57 of file base_sweeper.cpp.

```
57                                                {
58     this -> print_info = print_info;
59 }
```

Here is the caller graph for this function:

4.14.3.10 set_save_data()

```
void BaseSweeper::set_save_data (
            bool save_data )  [inherited]
```

Definition at line 60 of file base_sweeper.cpp.

```
60                                          {
61     this -> save_data = save_data;
62 }
```

Here is the caller graph for this function:

4.14.4 Member Data Documentation

4.14.4.1 CUDA_use

```
bool BaseSweeper::CUDA_use  [protected], [inherited]
```

Definition at line 36 of file base_sweeper.h.

4.14.4.2 end

```
float BaseSweeper::end  [protected], [inherited]
```

Definition at line 25 of file base_sweeper.h.

4.14.4.3 endpoint

```
bool BaseSweeper::endpoint  [protected], [inherited]
```

Definition at line 27 of file base_sweeper.h.

4.14.4.4 gpu_limit

```
int BaseSweeper::gpu_limit =3  [protected], [inherited]
```

Definition at line 38 of file base_sweeper.h.

4.14.4.5 gpu_num

```
int BaseSweeper::gpu_num =1  [protected], [inherited]
```

Definition at line 37 of file base_sweeper.h.

4.14.4.6 MPI_use

```
bool BaseSweeper::MPI_use  [protected], [inherited]
```

Definition at line 34 of file base_sweeper.h.

4.14.4.7 num

```
int BaseSweeper::num  [protected], [inherited]
```

Definition at line 26 of file base_sweeper.h.

4.14.4.8 num_list

```
vector<float> BaseSweeper::num_list  [protected], [inherited]
```

Definition at line 28 of file base_sweeper.h.

4.14.4.9 print_info

```
bool BaseSweeper::print_info =true  [protected], [inherited]
```

Definition at line 40 of file base_sweeper.h.

4.14.4.10 rank

```
int BaseSweeper::rank =0  [protected], [inherited]
```

Definition at line 32 of file base_sweeper.h.

4.14.4.11 save_data

```
bool BaseSweeper::save_data =true  [protected], [inherited]
```

Definition at line 41 of file base_sweeper.h.

4.14.4.12 size

```
int BaseSweeper::size =0  [protected], [inherited]
```

Definition at line 33 of file base_sweeper.h.

4.14.4.13 start

```
float BaseSweeper::start  [protected], [inherited]
```

Definition at line 24 of file base_sweeper.h.

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

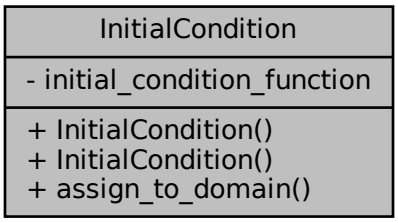
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/sweeper/harmonic_p_sweeper.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/sweeper/harmonic_p_sweeper.cpp

4.15 InitialCondition Class Reference

Initial condition class.

`#include <initial_condition.h>`

Collaboration diagram for InitialCondition:



Public Member Functions

- InitialCondition ()=default
- InitialCondition (std::function< std::complex< float >(float, float)> initial_condition_function)
  Construct a new Initial Condition:: Initial Condition object.
- void assign_to_domain (RectangularDomain *domain)
  Assign initial condition to the domain class instance.

Private Attributes

- std::function< std::complex< float >float, float)> initial_condition_function

4.15.1 Detailed Description

Initial condition class.

Definition at line 24 of file initial_condition.h.

4.15.2 Constructor & Destructor Documentation

4.15.2.1 InitialCondition() [1/2]

```
InitialCondition::InitialCondition ( )  [default]
```

4.15.2.2 InitialCondition() [2/2]

```
InitialCondition::InitialCondition (
            std::function< std::complex< float >(float, float)> initial_condition_function )
```

Construct a new Initial Condition:: Initial Condition object.

Parameters

initial_condition_function	

Definition at line 18 of file initial_condition.cpp.

```
19 {
20     this->initial_condition_function = initial_condition_function;
21 }
```

4.15.3 Member Function Documentation

4.15.3.1 assign_to_domain()

```
void InitialCondition::assign_to_domain (
            RectangularDomain * domain )
```

Assign initial condition to the domain class instance.

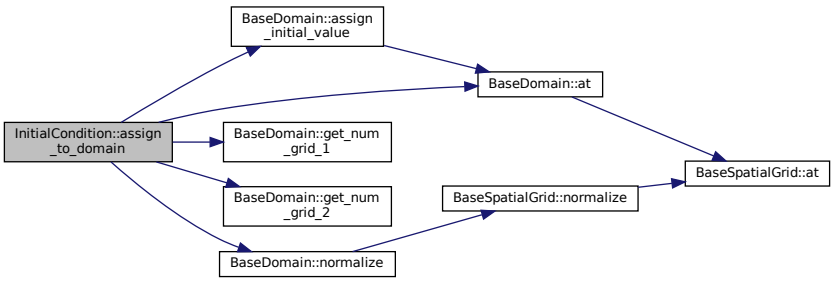
Parameters

domain	

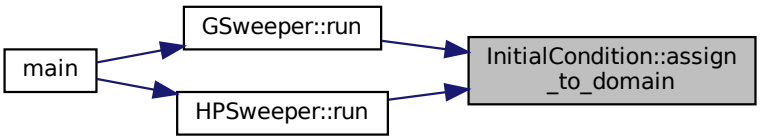
Definition at line 28 of file initial_condition.cpp.

```
29 {
30
31     for (auto i = 0; i < domain->get_num_grid_1(); ++i)
32     {
33         for (auto j = 0; j < domain->get_num_grid_2(); ++j)
34         {
35             auto point_data = domain->at(i, j, 0);
36             domain->assign_initial_value(i, j, this->initial_condition_function(point_data->x,
    point_data->y));
37         }
38     }
39     domain->normalize(0);
40 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.15.4 Member Data Documentation

4.15.4.1 initial_condition_function

```
std::function<std::complex<float>float, float)> InitialCondition::initial_condition_function
[private]
```

Definition at line 27 of file initial_condition.h.

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

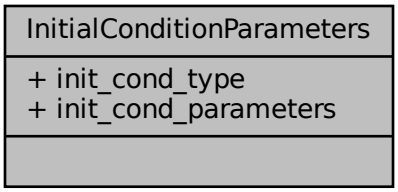
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/initial_condition/initial_condition.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/initial_condition/initial_condition.cpp

4.16 InitialConditionParameters Class Reference

Initial condition branch parameters containing information about initial condition.

```
#include <parameters.h>
```

Collaboration diagram for InitialConditionParameters:



Public Attributes

- std::string init_cond_type = std::string("")
- std::map< std::string, float > init_cond_parameters

4.16.1 Detailed Description

Initial condition branch parameters containing information about initial condition.

Definition at line 46 of file parameters.h.

4.16.2 Member Data Documentation

4.16.2.1 init_cond_parameters

```
std::map<std::string, float> InitialConditionParameters::init_cond_parameters
```

Definition at line 50 of file parameters.h.

4.16.2.2 init_cond_type

```
std::string InitialConditionParameters::init_cond_type = std::string("")
```

Definition at line 49 of file parameters.h.

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

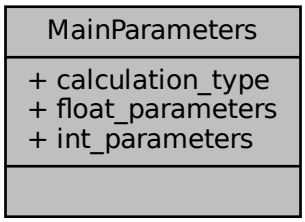
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/parameters.h

4.17 MainParameters Class Reference

Main branch parameters containing information about overall calculation.

```
#include <parameters.h>
```

Collaboration diagram for MainParameters:



Public Attributes

- std::string calculation_type = std::string("")
- std::map< std::string, float > float_parameters
- std::map< std::string, int > int_parameters

4.17.1 Detailed Description

Main branch parameters containing information about overall calculation.

Definition at line 21 of file parameters.h.

4.17.2 Member Data Documentation

4.17.2.1 calculation_type

```
std::string MainParameters::calculation_type = std::string("")
```

Definition at line 24 of file parameters.h.

4.17.2.2 float_parameters

```
std::map<std::string, float> MainParameters::float_parameters
```

Definition at line 25 of file parameters.h.

4.17.2.3 int_parameters

```
std::map<std::string, int> MainParameters::int_parameters
```

Definition at line 26 of file parameters.h.

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

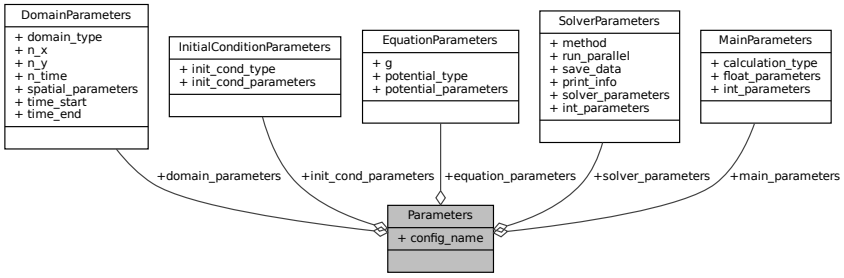
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/parameters.h

4.18 Parameters Class Reference

Parameters containing configuration name and all other branched parameters.

`#include <parameters.h>`

Collaboration diagram for Parameters:



Public Attributes

- std::string config_name
- MainParameters main_parameters
- DomainParameters domain_parameters
- InitialConditionParameters init_cond_parameters
- EquationParameters equation_parameters
- SolverParameters solver_parameters

4.18.1 Detailed Description

Parameters containing configuration name and all other branched parameters.

Definition at line 84 of file parameters.h.

4.18.2 Member Data Documentation

4.18.2.1 config_name

`std::string Parameters::config_name`

Definition at line 87 of file parameters.h.

4.18.2.2 domain_parameters

```
DomainParameters Parameters::domain_parameters
```

Definition at line 89 of file parameters.h.

4.18.2.3 equation_parameters

```
EquationParameters Parameters::equation_parameters
```

Definition at line 91 of file parameters.h.

4.18.2.4 init_cond_parameters

```
InitialConditionParameters Parameters::init_cond_parameters
```

Definition at line 90 of file parameters.h.

4.18.2.5 main_parameters

```
MainParameters Parameters::main_parameters
```

Definition at line 88 of file parameters.h.

4.18.2.6 solver_parameters

```
SolverParameters Parameters::solver_parameters
```

Definition at line 92 of file parameters.h.

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

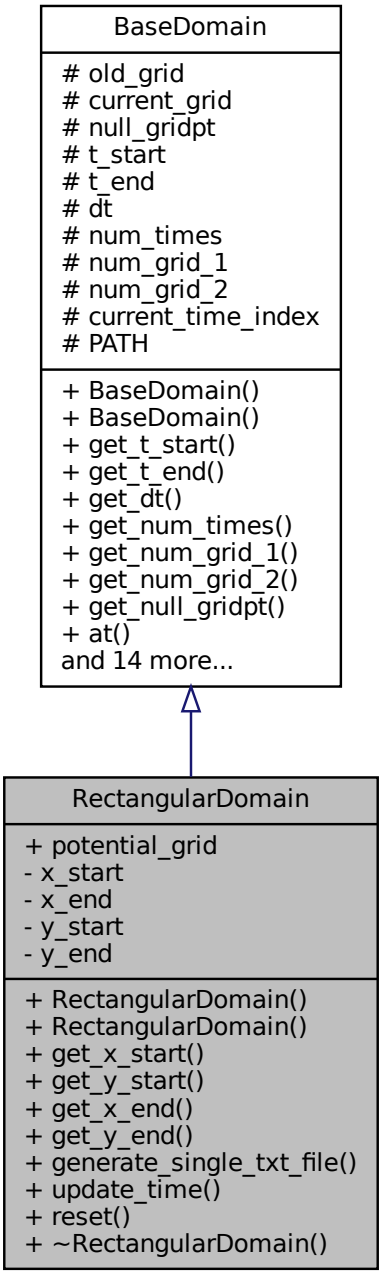
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/parameters.h

4.19 RectangularDomain Class Reference

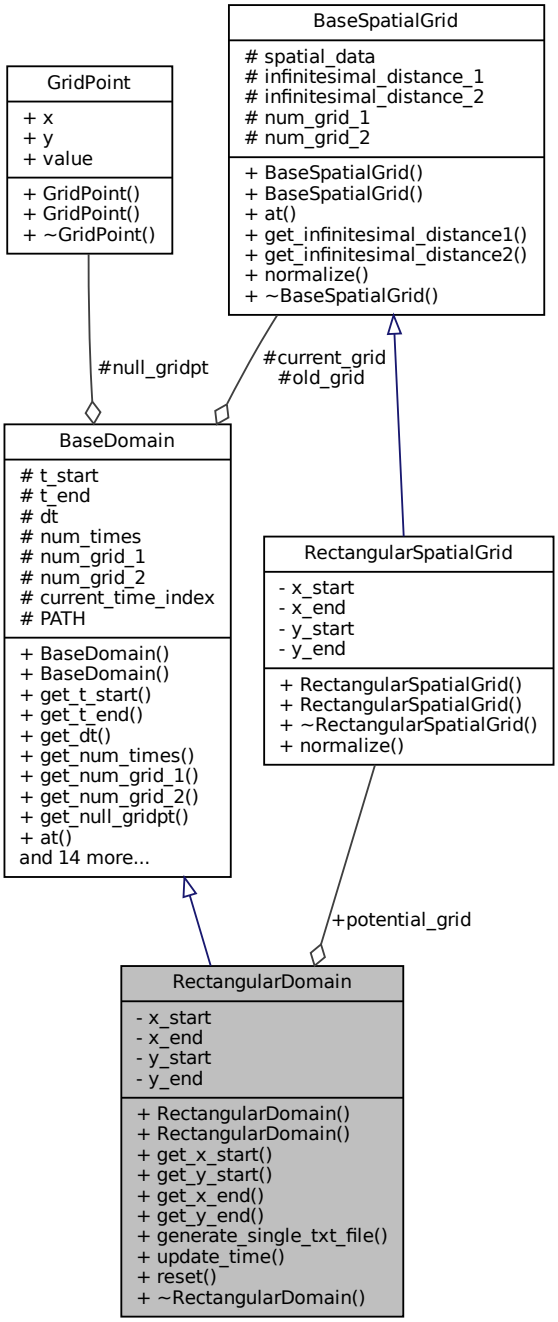
Rectangular domain containing multiple timesteps.

`#include <rect_domain.h>`

Inheritance diagram for RectangularDomain:



Collaboration diagram for RectangularDomain:



Public Member Functions

- RectangularDomain ()=default
- RectangularDomain (int num_grid_1, int num_grid_2, float t_start, float t_end, int num_times, float x_start, float x_end, float y_start, float y_end)

  Construct a new Rectangular Domain:: Rectangular Domain object.
- float get_x_start ()

- float get_y_start ()
- float get_x_end ()
- float get_y_end ()
- void generate_single_txt_file (std::string filename, bool cuda_mode=false)
- void update_time (bool cuda_mode=false)
- void reset ()
- ~RectangularDomain ()
- float get_t_start ()
- float get_t_end ()
- float get_dt ()
- int get_num_times ()
- int get_num_grid_1 ()
- int get_num_grid_2 ()
- GridPoint * get_null_gridpt ()
- GridPoint * at (int index_1, int index_2, int time_index)
- void assign_initial_value (int index_1, int index_2, std::complex< float > value)

  Assign initial value.
- void assign_wave_function (int index_1, int index_2, int time_index, std::complex< float > value)
- float time_at (int time_index)
- float get_infinitesimal_distance1 ()
- float get_infinitesimal_distance2 ()
- void generate_directory_name (std::string info, bool print_info=true)

  create directory and return directory name with "/" directory name : "./results/%d-%m-%Y %H-%M-%S_"+info for exmaple, "./results/"
- void normalize (int time_index)
- void print_directory_info ()
- int get_current_time_index ()
- std::string get_path ()

Public Attributes

- RectangularSpatialGrid * potential_grid

Protected Attributes

- BaseSpatialGrid * old_grid
- BaseSpatialGrid * current_grid
- GridPoint * null_gridpt
- float t_start
- float t_end
- float dt
- int num_times
- int num_grid_1
- int num_grid_2
- int current_time_index = 0
- std::string PATH

Private Attributes

- float x_start
- float x_end
- float y_start
- float y_end

4.19.1 Detailed Description

Rectangular domain containing multiple timesteps.

Definition at line 37 of file rect_domain.h.

4.19.2 Constructor & Destructor Documentation

4.19.2.1 RectangularDomain() [1/2]

```
RectangularDomain::RectangularDomain ( )  [default]
```

4.19.2.2 RectangularDomain() [2/2]

```
RectangularDomain::RectangularDomain (
            int num_grid_1,
            int num_grid_2,
            float t_start,
            float t_end,
            int num_times,
            float x_start,
            float x_end,
            float y_start,
            float y_end )
```

Construct a new Rectangular Domain:: Rectangular Domain object.

Parameters

num_grid_1	Number of grids in x axis
num_grid_2	Number of grids in y axis
t_start	Initial time
t_end	Final time
num_times	iteration number or number of time points
x_start	Start point of x axis
x_end	End point of x axis
y_start	Start point of y axis
y_end	Start point of x axis

Definition at line 92 of file rect_domain.cpp.

```
103     : BaseDomain(num_grid_1, num_grid_2, t_start, t_end, num_times),
104       x_start(x_start),
105       x_end(x_end),
106       y_start(y_start),
```

```
107       y_end(y_end)
108 {
109
110     delete (this->old_grid);
111     delete (this->current_grid);
112     this->old_grid = new RectangularSpatialGrid(num_grid_1, num_grid_2, x_start, x_end, y_start, y_end);
113     this->current_grid = new RectangularSpatialGrid(num_grid_1, num_grid_2, x_start, x_end, y_start,
      y_end);
114     this->potential_grid = new RectangularSpatialGrid(num_grid_1, num_grid_2, x_start, x_end, y_start,
      y_end);
115 };
```

4.19.2.3 ~RectangularDomain()

```
RectangularDomain::~RectangularDomain ( )
```

Definition at line 116 of file rect_domain.cpp.

```
117 {
118     delete this->potential_grid;
119 };
```

4.19.3 Member Function Documentation

4.19.3.1 assign_initial_value()

```
void BaseDomain::assign_initial_value (
            int index_1,
            int index_2,
            std::complex< float > value )  [inherited]
```

Assign initial value.

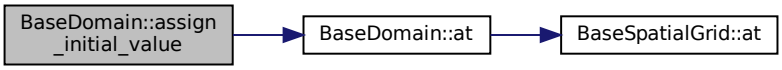
Parameters

index_1	x = x_start + index_1∗dx
index_2	y = y_start + index_2 ∗ dy
value	initial value at x, y

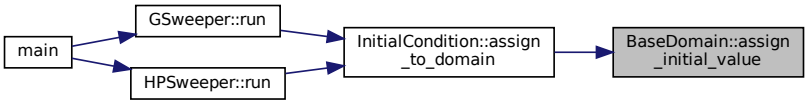
Definition at line 188 of file base_domain.cpp.

```
189 {
190     this->at(index_1, index_2, 0)->value = value;
191 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



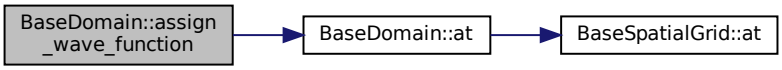
4.19.3.2 assign_wave_function()

```
void BaseDomain::assign_wave_function (
            int index_1,
            int index_2,
            int time_index,
            std::complex< float > value )  [inherited]
```

Definition at line 192 of file base_domain.cpp.

```
193 {
194     this->at(index_1, index_2, time_index)->value = value;
195 }
```

Here is the call graph for this function:



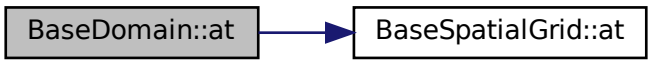
4.19.3.3 at()

```
GridPoint * BaseDomain::at (
            int index_1,
            int index_2,
            int time_index )  [inherited]
```

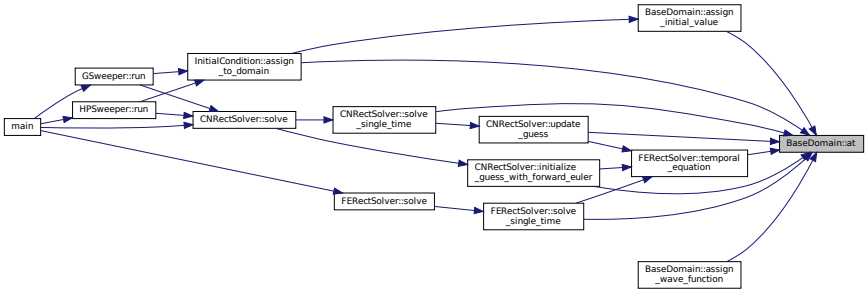
Definition at line 153 of file base_domain.cpp.

```
154 {
155     if (time_index == this->current_time_index)
156     {
157         return this->current_grid->at(index_1, index_2);
158     }
159     else if (time_index == this->current_time_index - 1)
160     {
161         return this->old_grid->at(index_1, index_2);
162     }
163     else
164     {
165         std::cerr << "error in base domin at function" << std::endl;
166         return this->current_grid->at(index_1, index_2);
167     }
168 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.19.3.4 generate_directory_name()

```
void BaseDomain::generate_directory_name (
            std::string info,
            bool print_info = true )  [inherited]
```

create directory and return directory name with "/" directory name : "./results/%d-%m-%Y %H-%M-%S_"+info for exmaple, "./results/"

Parameters

info	information about domain type and solver type

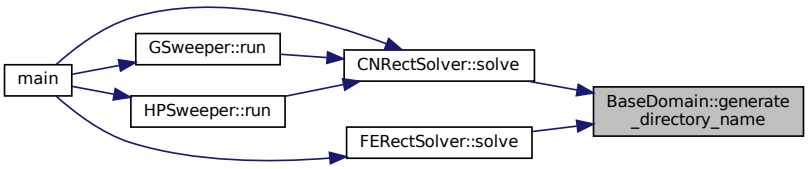
Returns

std::string directory name with "/"

Definition at line 203 of file base_domain.cpp.

```
204 {
205     auto t = std::time(nullptr);
206     auto tm = *std::localtime(&t);
207 
208     std::ostringstream oss;
209     oss << std::put_time(&tm, "%Y-%m-%d-%H-%M-%S");
210     auto str = oss.str();
211     std::string directory_name = "../results/" + str + "_" + info;
212     bool created = fs::create_directory(directory_name.c_str());
213     if (print_info && created)
214     {
215         std::cout << "Created directory " << directory_name << std::endl;
216     }
217     // else if(print_info )
218     //TODO
219     else if (!created)
220     {
221         std::cout << "Creating directory failed" << std::endl;
222     }
223 
224     this->PATH = directory_name + "/";
225 }
```

Here is the caller graph for this function:



4.19.3.5 generate_single_txt_file()

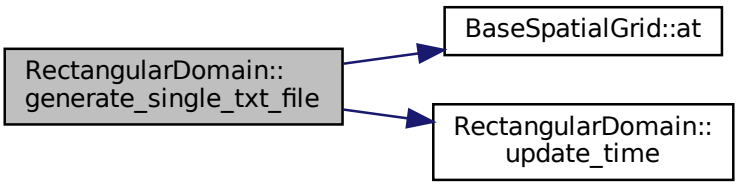
```
void RectangularDomain::generate_single_txt_file (
            std::string filename,
            bool cuda_mode = false )
```

Definition at line 152 of file rect_domain.cpp.

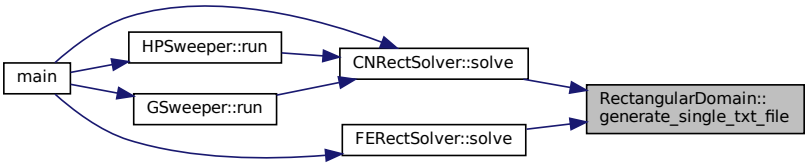
```
153 {
154     if (cuda_mode)
155     {
156         this->update_time(cuda_mode);
157     }
158     else
159     {
160         std::ofstream outfile(this->PATH + filename + ".txt");
161         outfile << "x, y, real, imag, magn, phase " << std::endl;
162         for (auto i = 0; i < num_grid_1; ++i)
163         {
```

```
164             for (auto j = 0; j < num_grid_2; ++j)
165             {
166                 float magnitude = std::abs(this->current_grid->at(i, j)->value);
167                 float phase = std::arg(this->current_grid->at(i, j)->value);
168                 outfile « this->current_grid->at(i, j)->x « ", " « this->current_grid->at(i, j)->y « ",
    ";
169                 outfile « this->current_grid->at(i, j)->value.real() « ", " « this->current_grid->at(i,
    j)->value.imag() « ", ";
170                 outfile « magnitude « ", " « phase;
171                 outfile « std::endl;
172             }
173         }
174         outfile.close();
175         // After saving data, update domain
176         this->update_time();
177     }
178 };
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.19.3.6 get_current_time_index()

```
int BaseDomain::get_current_time_index ( )  [inherited]
```

Definition at line 170 of file base_domain.cpp.

```
171 {
172     return this->current_time_index;
173 }
```

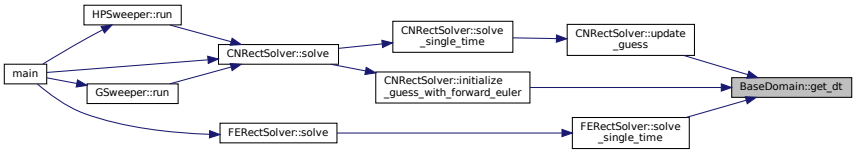
4.19.3.7 get_dt()

```
float BaseDomain::get_dt ( )  [inherited]
```

Definition at line 125 of file base_domain.cpp.

```
126 {
127     return this->dt;
128 }
```

Here is the caller graph for this function:



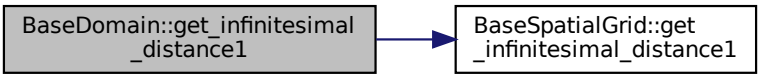
4.19.3.8 get_infinitesimal_distance1()

```
float BaseDomain::get_infinitesimal_distance1 ( )  [inherited]
```

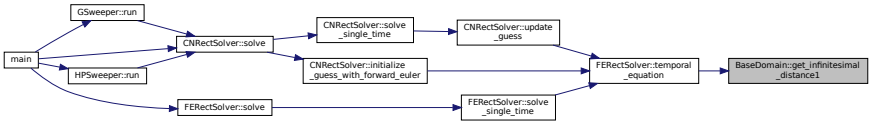
Definition at line 143 of file base_domain.cpp.

```
144 {
145     return this->old_grid->get_infinitesimal_distance1();
146 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



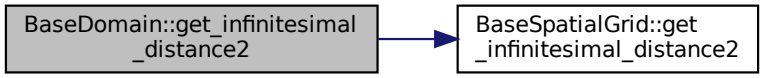
4.19.3.9 get_infinitesimal_distance2()

```
float BaseDomain::get_infinitesimal_distance2 ( )  [inherited]
```

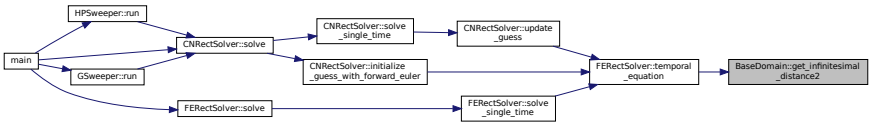
Definition at line 147 of file base_domain.cpp.

```
148 {
149     return this->old_grid->get_infinitesimal_distance2();
150 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



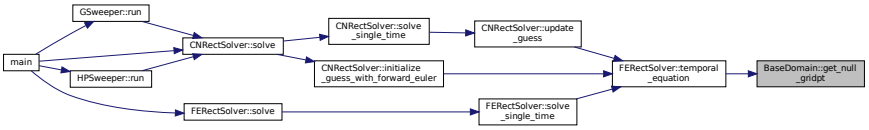
4.19.3.10 get_null_gridpt()

```
GridPoint * BaseDomain::get_null_gridpt ( )  [inherited]
```

Definition at line 176 of file base_domain.cpp.

```
177 {
178     return this->null_gridpt;
179 }
```

Here is the caller graph for this function:



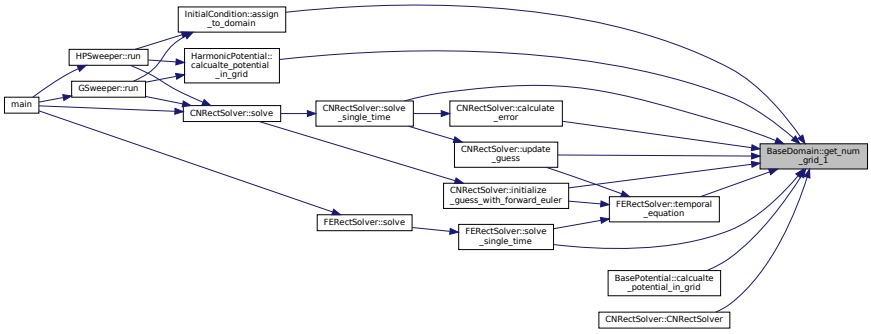
4.19.3.11 get_num_grid_1()

```
int BaseDomain::get_num_grid_1 ( )  [inherited]
```

Definition at line 134 of file base_domain.cpp.

```
135 {
136     return this->num_grid_1;
137 }
```

Here is the caller graph for this function:



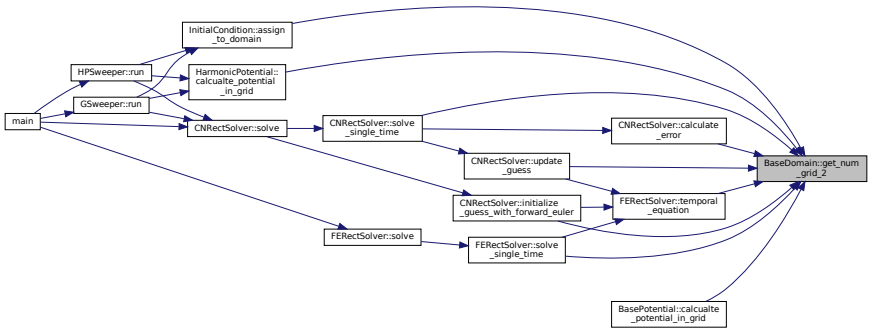
4.19.3.12 get_num_grid_2()

```
int BaseDomain::get_num_grid_2 ( )  [inherited]
```

Definition at line 138 of file base_domain.cpp.

```
139 {
140     return this->num_grid_2;
141 }
```

Here is the caller graph for this function:



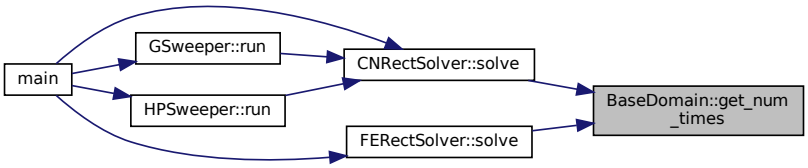
4.19.3.13 get_num_times()

```
int BaseDomain::get_num_times ( )  [inherited]
```

Definition at line 129 of file base_domain.cpp.

```
130 {
131     return this->num_times;
132 }
```

Here is the caller graph for this function:



4.19.3.14 get_path()

```
std::string BaseDomain::get_path ( )  [inherited]
```

Definition at line 106 of file base_domain.cpp.

```
107 {
108     return this->PATH;
109 }
```

4.19.3.15 get_t_end()

```
float BaseDomain::get_t_end ( )  [inherited]
```

Definition at line 121 of file base_domain.cpp.

```
122 {
123     return this->t_end;
124 }
```

4.19.3.16 get_t_start()

```
float BaseDomain::get_t_start ( )  [inherited]
```

Definition at line 116 of file base_domain.cpp.

```
117 {
118     return this->t_start;
119 }
```

4.19.3.17 get_x_end()

```
float RectangularDomain::get_x_end ( )
```

Definition at line 128 of file rect_domain.cpp.

```
129 {
130     return this->x_end;
131 }
```

4.19.3.18 get_x_start()

```
float RectangularDomain::get_x_start ( )
```

Definition at line 120 of file rect_domain.cpp.

```
121 {
122     return this->x_start;
123 }
```

4.19.3.19 get_y_end()

```
float RectangularDomain::get_y_end ( )
```

Definition at line 132 of file rect_domain.cpp.

```
133 {
134     return this->x_end;
135 }
```

4.19.3.20 get_y_start()

```
float RectangularDomain::get_y_start ( )
```

Definition at line 124 of file rect_domain.cpp.

```
125 {
126     return this->y_start;
127 }
```

4.19.3.21 normalize()

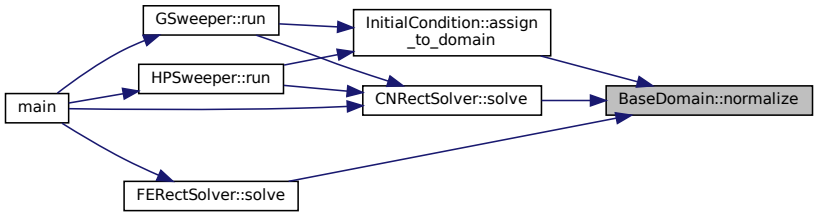
```
void BaseDomain::normalize (
            int time_index )  [inherited]
```

Definition at line 111 of file base_domain.cpp.

```
112 {
113     this->current_grid->normalize();
114 }
```

Here is the call graph for this function:

Here is the caller graph for this function:



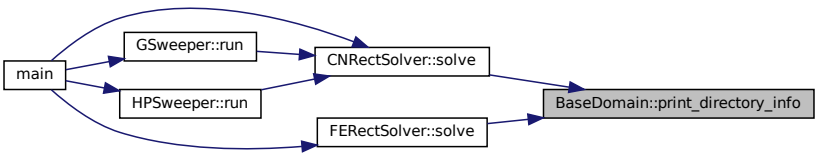
4.19.3.22 print_directory_info()

```
void BaseDomain::print_directory_info ( )  [inherited]
```

Definition at line 261 of file base_domain.cpp.

```
262 {
263     std::cout « this->num_times;
264     std::cout « " text files are generated in \n";
265     std::cout « this->PATH « std::endl;
266 }
```

Here is the caller graph for this function:



4.19.3.23 reset()

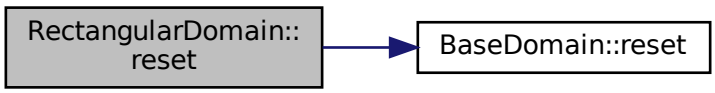
```
void RectangularDomain::reset ( )  [virtual]
```

Reimplemented from BaseDomain.

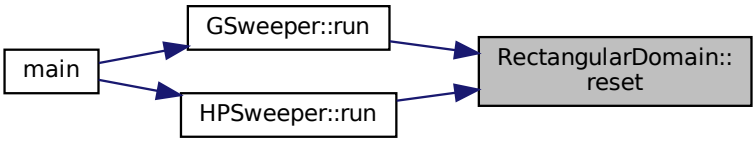
Definition at line 180 of file rect_domain.cpp.

```
181 {
182     BaseDomain::reset();
183     delete this->potential_grid;
184 
185     this->old_grid = new RectangularSpatialGrid(num_grid_1, num_grid_2, x_start, x_end, y_start, y_end);
186     this->current_grid = new RectangularSpatialGrid(num_grid_1, num_grid_2, x_start, x_end, y_start,
      y_end);
187     this->potential_grid = new RectangularSpatialGrid(num_grid_1, num_grid_2, x_start, x_end, y_start,
      y_end);
188 
189 }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.19.3.24 time_at()

```
float BaseDomain::time_at (
            int time_index )  [inherited]
```

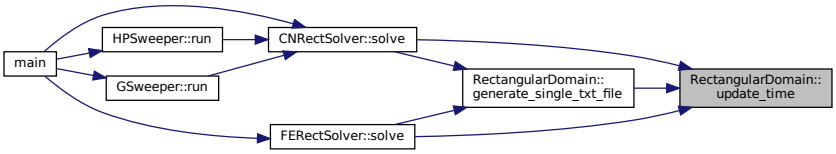
4.19.3.25 update_time()

```
void RectangularDomain::update_time (
            bool cuda_mode = false )
```

Definition at line 137 of file rect_domain.cpp.

```
138 {
139     if (cuda_mode)
140     {
141         this->current_time_index += 1;
142     }
143     else
144     {
145         this->current_time_index += 1;
146         delete (this->old_grid);
147         this->old_grid = this->current_grid;
148         this->current_grid = new RectangularSpatialGrid(num_grid_1, num_grid_2, x_start, x_end, y_start,
      y_end);
149     }
150 }
```

Here is the caller graph for this function:



4.19.4 Member Data Documentation

4.19.4.1 current_grid

```
BaseSpatialGrid* BaseDomain::current_grid  [protected], [inherited]
```

Definition at line 98 of file base_domain.h.

4.19.4.2 current_time_index

```
int BaseDomain::current_time_index = 0  [protected], [inherited]
```

Definition at line 102 of file base_domain.h.

4.19.4.3 dt

```
float BaseDomain::dt  [protected], [inherited]
```

Definition at line 100 of file base_domain.h.

4.19.4.4 null_gridpt

```
GridPoint* BaseDomain::null_gridpt  [protected], [inherited]
```

Definition at line 99 of file base_domain.h.

4.19.4.5 num_grid_1

```
int BaseDomain::num_grid_1  [protected], [inherited]
```

Definition at line 101 of file base_domain.h.

4.19.4.6 num_grid_2

```
int BaseDomain::num_grid_2  [protected], [inherited]
```

Definition at line 101 of file base_domain.h.

4.19.4.7 num_times

```
int BaseDomain::num_times  [protected], [inherited]
```

Definition at line 101 of file base_domain.h.

4.19.4.8 old_grid

```
BaseSpatialGrid* BaseDomain::old_grid  [protected], [inherited]
```

Definition at line 97 of file base_domain.h.

4.19.4.9 PATH

```
std::string BaseDomain::PATH  [protected], [inherited]
```

Definition at line 103 of file base_domain.h.

4.19.4.10 potential_grid

```
RectangularSpatialGrid* RectangularDomain::potential_grid
```

Definition at line 48 of file rect_domain.h.

4.19.4.11 t_end

```
float BaseDomain::t_end  [protected], [inherited]
```

Definition at line 100 of file base_domain.h.

4.19.4.12 t_start

```
float BaseDomain::t_start  [protected], [inherited]
```

Definition at line 100 of file base_domain.h.

4.19.4.13 x_end

```
float RectangularDomain::x_end  [private]
```

Definition at line 55 of file rect_domain.h.

4.19.4.14 x_start

```
float RectangularDomain::x_start  [private]
```

Definition at line 54 of file rect_domain.h.

4.19.4.15 y_end

```
float RectangularDomain::y_end  [private]
```

Definition at line 57 of file rect_domain.h.

4.19.4.16 y_start

```
float RectangularDomain::y_start  [private]
```

Definition at line 56 of file rect_domain.h.

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

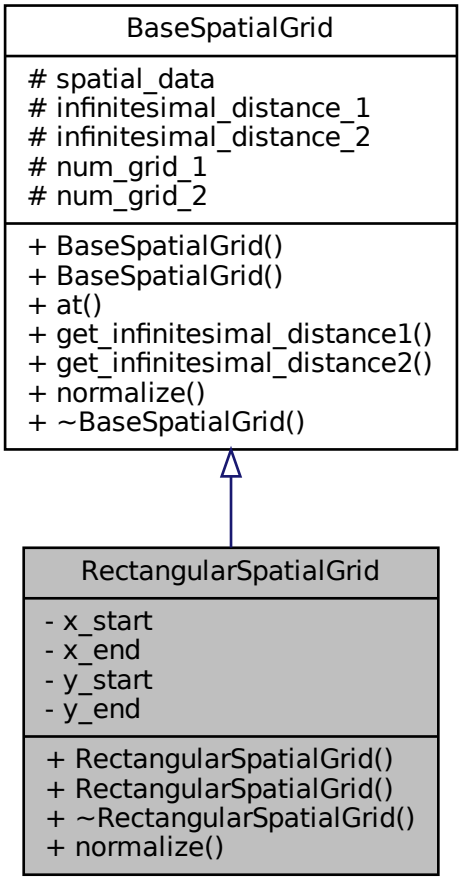
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/domain/rect_domain.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/domain/rect_domain.cpp

4.20 RectangularSpatialGrid Class Reference

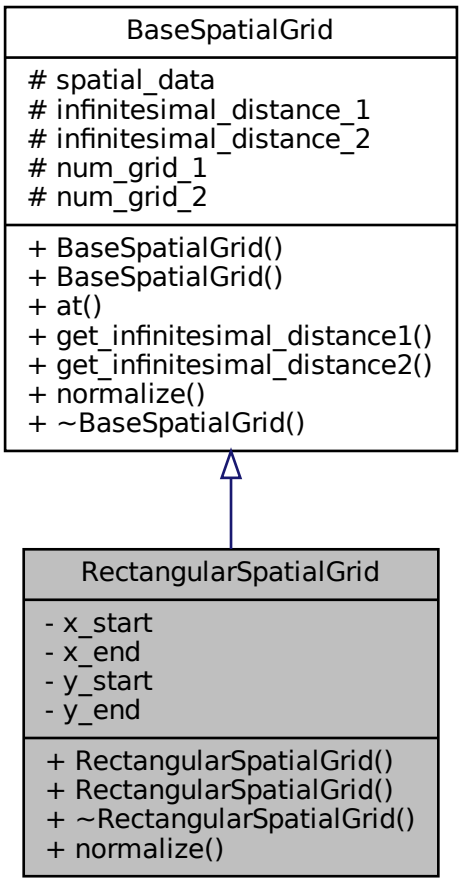
Rectangular Spatial Grid class for single time step.

```
#include <rect_domain.h>
```

Inheritance diagram for RectangularSpatialGrid:



Collaboration diagram for RectangularSpatialGrid:



Public Member Functions

- RectangularSpatialGrid ()=default
- RectangularSpatialGrid (int num_grid_1, int num_grid_2, float x_start, float x_end, float y_start, float y_end)

  Construct a new Rectangular Spatial Grid:: Rectangular Spatial Grid object.
- ~RectangularSpatialGrid ()
- void normalize ()
- GridPoint * at (int index_1, int index_2)
- float get_infinitesimal_distance1 ()
- float get_infinitesimal_distance2 ()

Protected Attributes

- std::vector< std::vector< GridPoint > > spatial_data
- float infinitesimal_distance_1
- float infinitesimal_distance_2
- int num_grid_1
- int num_grid_2

Private Attributes

- float x_start
- float x_end
- float y_start
- float y_end

4.20.1 Detailed Description

Rectangular Spatial Grid class for single time step.

Definition at line 18 of file rect_domain.h.

4.20.2 Constructor & Destructor Documentation

4.20.2.1 RectangularSpatialGrid() [1/2]

```
RectangularSpatialGrid::RectangularSpatialGrid ( )  [default]
```

4.20.2.2 RectangularSpatialGrid() [2/2]

```
RectangularSpatialGrid::RectangularSpatialGrid (
            int num_grid_1,
            int num_grid_2,
            float x_start,
            float x_end,
            float y_start,
            float y_end )
```

Construct a new Rectangular Spatial Grid:: Rectangular Spatial Grid object.

Parameters

num_grid_1	Number of grids in x axis
num_grid_2	Number of grids in y axis
x_start	Start point of x axis
x_end	End point of x axis
y_start	Start point of y axis
y_end	Start point of x axis

Definition at line 26 of file rect_domain.cpp.

```
32                 : BaseSpatialGrid(num_grid_1, num_grid_2)
```

```
33 {
34     this->x_start = x_start;
35     this->x_end = x_end;
36     this->y_start = y_start;
37     this->y_end = y_end;
38     //infinitesimal_distance 1,2 = dx, dy
39     this->infinitesimal_distance_1 = (x_end - x_start) / (num_grid_1 - 1);
40     this->infinitesimal_distance_2 = (y_end - y_start) / (num_grid_2 - 1);
41     //For each GridPoint, set x, y position. Also, set wave_function as 0+0i default value
42     for (auto i = 0; i < num_grid_1; ++i)
43     {
44         for (auto j = 0; j < num_grid_2; ++j)
45         {
46             this->spatial_data[i][j] = GridPoint(this->x_start + infinitesimal_distance_1 * i,
47                                                  this->y_start + infinitesimal_distance_2 * j,
48                                                  //{real value, imaginary value}
49                                                  std::complex<float>{0, 0});
50         }
51     }
52 }
```

4.20.2.3 ~RectangularSpatialGrid()

```
RectangularSpatialGrid::~RectangularSpatialGrid ( )
```

Definition at line 76 of file rect_domain.cpp.

```
76                                                  {
77
78 };
```

4.20.3 Member Function Documentation

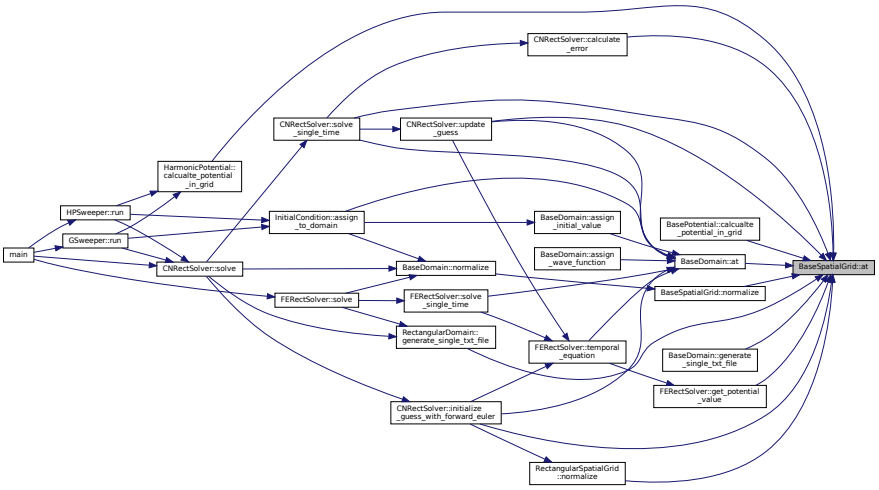
4.20.3.1 at()

```
GridPoint * BaseSpatialGrid::at (
            int index_1,
            int index_2 )  [inherited]
```

Definition at line 76 of file base_domain.cpp.

```
77 {
78     return &this->spatial_data[index_1 % this->num_grid_1][index_2 % this->num_grid_2];
79 }
```

Here is the caller graph for this function:



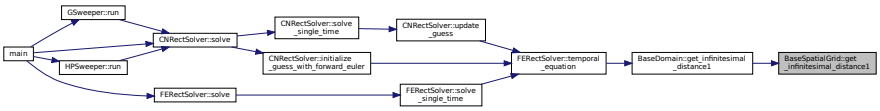
4.20.3.2 get_infinitesimal_distance1()

```
float BaseSpatialGrid::get_infinitesimal_distance1 ( )  [inherited]
```

Definition at line 64 of file base_domain.cpp.

```
65 {
66     return this->infinitesimal_distance_1;
67 }
```

Here is the caller graph for this function:



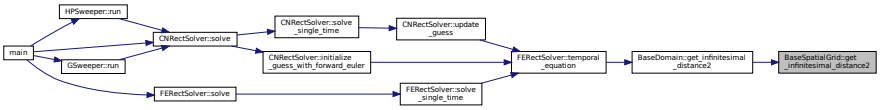
4.20.3.3 get_infinitesimal_distance2()

```
float BaseSpatialGrid::get_infinitesimal_distance2 ( )  [inherited]
```

Definition at line 70 of file base_domain.cpp.

```
71 {
72     return this->infinitesimal_distance_2;
73 }
```

Here is the caller graph for this function:



4.20.3.4 normalize()

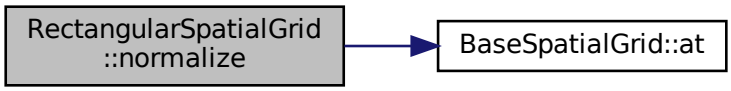
```
void RectangularSpatialGrid::normalize ( )
```

Definition at line 53 of file rect_domain.cpp.

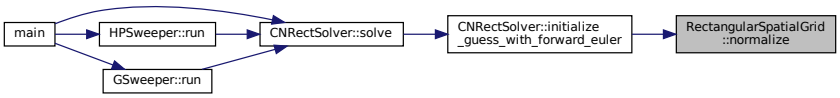
```
54 {
55     float sum = 0.;
56     for (auto i = 0; i < this->num_grid_1; ++i)
57     {
58         for (auto j = 0; j < this->num_grid_2; ++j)
59         {
60             auto wave_func = this->at(i, j)->value;
61             sum += float(std::pow(std::abs(wave_func), 2));
62         }
63     }
```

```
64      sum = std::sqrt(sum * this->infinitesimal_distance_1 * this->infinitesimal_distance_2);
65      for (auto i = 0; i < this->num_grid_1; ++i)
66      {
67          for (auto j = 0; j < this->num_grid_2; ++j)
68          {
69              this->at(i, j)->value /= sum;
70          }
71      }
72
73  }
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.20.4 Member Data Documentation

4.20.4.1 infinitesimal_distance_1

`float BaseSpatialGrid::infinitesimal_distance_1 [protected], [inherited]`

Definition at line 59 of file base_domain.h.

4.20.4.2 infinitesimal_distance_2

`float BaseSpatialGrid::infinitesimal_distance_2 [protected], [inherited]`

Definition at line 59 of file base_domain.h.

4.20.4.3 num_grid_1

```
int BaseSpatialGrid::num_grid_1  [protected], [inherited]
```

Definition at line 60 of file base_domain.h.

4.20.4.4 num_grid_2

```
int BaseSpatialGrid::num_grid_2  [protected], [inherited]
```

Definition at line 60 of file base_domain.h.

4.20.4.5 spatial_data

```
std::vector<std::vector<GridPoint> > BaseSpatialGrid::spatial_data  [protected], [inherited]
```

Definition at line 58 of file base_domain.h.

4.20.4.6 x_end

```
float RectangularSpatialGrid::x_end  [private]
```

Definition at line 28 of file rect_domain.h.

4.20.4.7 x_start

```
float RectangularSpatialGrid::x_start  [private]
```

Definition at line 27 of file rect_domain.h.

4.20.4.8 y_end

```
float RectangularSpatialGrid::y_end  [private]
```

Definition at line 30 of file rect_domain.h.

4.20.4.9 y_start

```
float RectangularSpatialGrid::y_start  [private]
```

Definition at line 29 of file rect_domain.h.

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

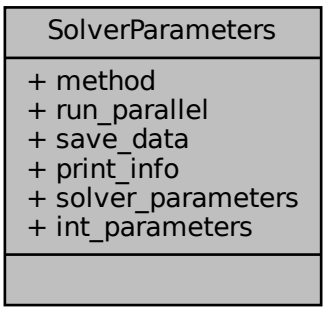
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/domain/rect_domain.h
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/domain/rect_domain.cpp

4.21 SolverParameters Class Reference

Solver branch parameters containing information about solver.

```
#include <parameters.h>
```

Collaboration diagram for SolverParameters:



Public Attributes

- std::string method = std::string("")
- bool run_parallel
- bool save_data
- bool print_info
- std::map< std::string, float > solver_parameters
- std::map< std::string, int > int_parameters

4.21.1 Detailed Description

Solver branch parameters containing information about solver.

Definition at line 69 of file parameters.h.

4.21.2 Member Data Documentation

4.21.2.1 int_parameters

```
std::map<std::string, int> SolverParameters::int_parameters
```

Definition at line 77 of file parameters.h.

4.21.2.2 method

```
std::string SolverParameters::method = std::string("")
```

Definition at line 72 of file parameters.h.

4.21.2.3 print_info

```
bool SolverParameters::print_info
```

Definition at line 75 of file parameters.h.

4.21.2.4 run_parallel

```
bool SolverParameters::run_parallel
```

Definition at line 73 of file parameters.h.

4.21.2.5 save_data

```
bool SolverParameters::save_data
```

Definition at line 74 of file parameters.h.

4.21.2.6 solver_parameters

```
std::map<std::string, float> SolverParameters::solver_parameters
```

Definition at line 76 of file parameters.h.

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

- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/parameters.h

Chapter 5

File Documentation

5.1 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/CMake↩ Lists.txt File Reference

Functions

- cmake_minimum_required (VERSION 3.5) enable_language(CUDA) file(GLOB_RECURSE SRC_FILES L↩ IST_DIRECTORIES false ∗.h ∗.cpp ∗.cu ∗cuh) find_package(MPI REQUIRED) include_directories($
- target_link_libraries (${BINARY}_run ${MPI_LIBRARIES}) target_link_libraries($

5.1.1 Function Documentation

5.1.1.1 cmake_minimum_required()

```
cmake_minimum_required (
             VERSION 3.  5 )
```

Definition at line 1 of file CMakeLists.txt.

```
4              {CMAKE_PROJECT_NAME} )
5 SET( EXECUTABLE_OUTPUT_PATH ${CMAKE_SOURCE_DIR}/build )
6 SET( LIBRARY_OUTPUT_PATH ${CMAKE_SOURCE_DIR}/build )
7
8 file(GLOB_RECURSE SRC_FILES LIST_DIRECTORIES false *.h *.cpp *.cu *cuh)
9 ADD_EXECUTABLE( ${BINARY}_run  ${SRC_FILES} )
10 ADD_LIBRARY( ${BINARY}_lib STATIC ${SRC_FILES} )
11
12 #MPI linking
13 find_package(MPI REQUIRED)
14 include_directories(${MPI_INCLUDE_PATH})
```

5.1.1.2 target_link_libraries()

```
target_link_libraries (
              ${BINARY}_run ${MPI_LIBRARIES} )
```

Definition at line 15 of file CMakeLists.txt.

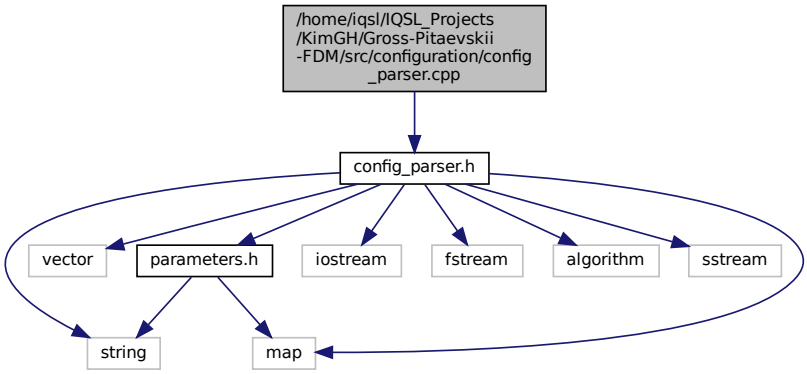
```
15                      {BINARY}_run ${MPI_LIBRARIES})
16 target_link_libraries(${BINARY}_lib ${MPI_LIBRARIES})
```

5.2 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/configuration/config_parser.cpp File Reference

Configuration Parser class implementation.

```
#include "config_parser.h"
```

Include dependency graph for config_parser.cpp:



5.2.1 Detailed Description

Configuration Parser class implementation.

Author

Gyeonghun Kim, Minyoung Kim

Version

0.1

Date

2022-06-09

Copyright

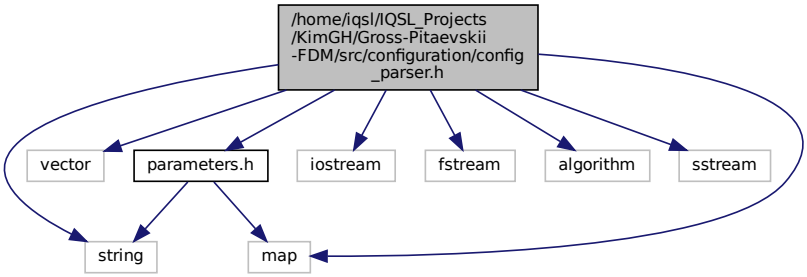
Copyright (c) 2022

5.3 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/config_parser.h File Reference

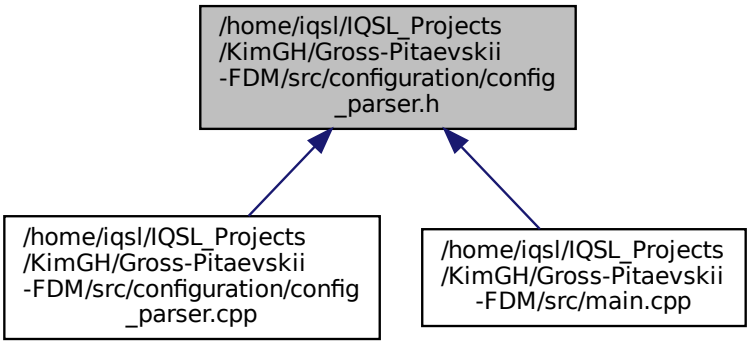
Configuration Parser Class header.

```
#include <string>
#include <vector>
#include <map>
#include <iostream>
#include <fstream>
#include <algorithm>
#include <sstream>
#include "parameters.h"
```

Include dependency graph for config_parser.h:



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



Classes

- class ConfigParser

  Configuration parser.

5.3.1 Detailed Description

Configuration Parser Class header.

Author

Gyeonghun Kim, Minyoung Kim

Version

0.1

Date

2022-06-09

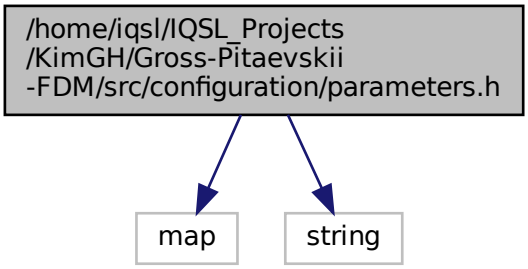
Copyright

5.4 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/parameters.h File Reference

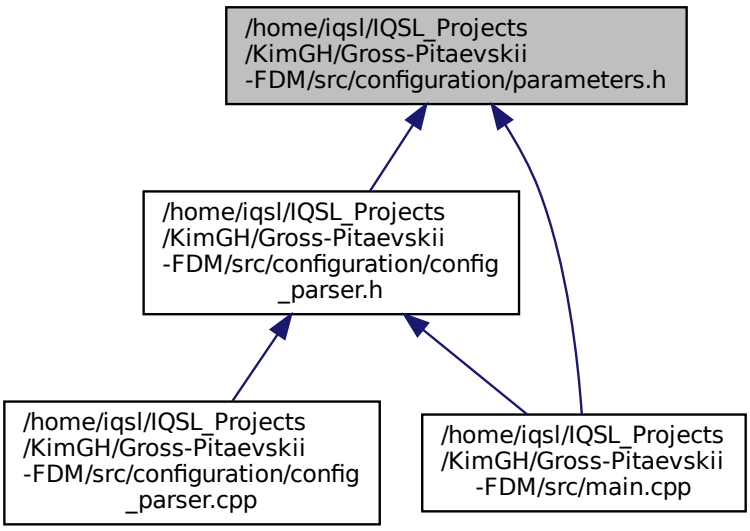
Header for the Parameter classes.

```
#include <map>
#include <string>
```

Include dependency graph for parameters.h:



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



Classes

- class MainParameters

  Main branch parameters containing information about overall calculation.
- class DomainParameters

  Domain branch parameters containing information about domain.
- class InitialConditionParameters

  Initial condition branch parameters containing information about initial condition.
- class EquationParameters

  Equation branch parameters containing information about equation.
- class SolverParameters

  Solver branch parameters containing information about solver.
- class Parameters

  Parameters containing configuration name and all other branched parameters.

5.4.1 Detailed Description

Header for the Parameter classes.

Author

Gyeonghun Kim, Minyoung Kim

Version

0.1

Date

2022-06-09

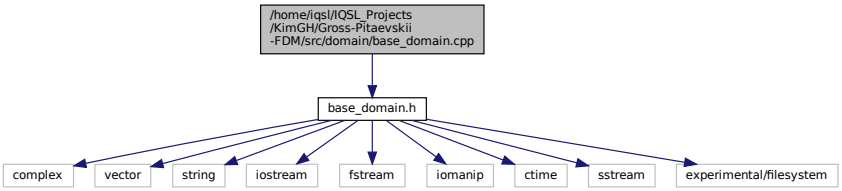
Copyright

5.5 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/domain/base_domain.cpp File Reference

Implementation of methods in the Base Domain class.

```
#include "base_domain.h"
```

Include dependency graph for base_domain.cpp:



5.5.1 Detailed Description

Implementation of methods in the Base Domain class.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-03

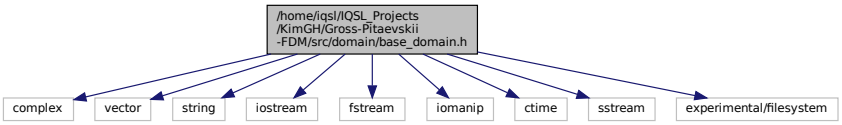
Copyright

5.6 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/domain/base_domain.h File Reference

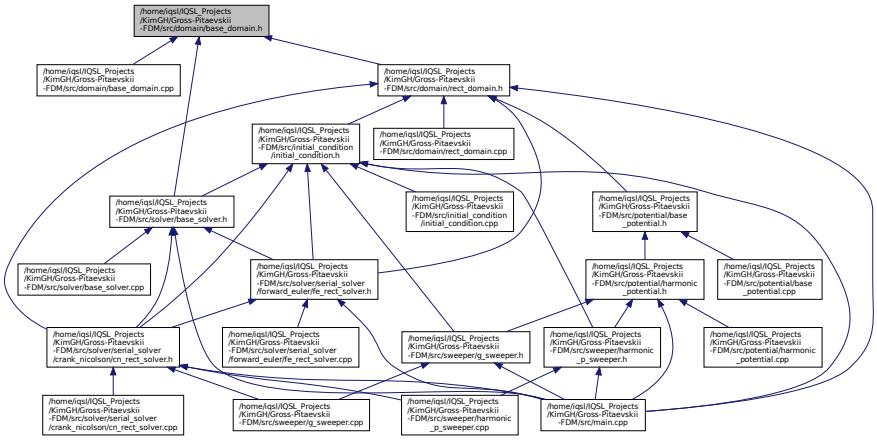
Header for Base domain class.

```
#include <complex>
#include <vector>
#include <string>
#include <iostream>
#include <fstream>
#include <iomanip>
#include <ctime>
#include <sstream>
#include <experimental/filesystem>
```

Include dependency graph for base_domain.h:



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



Classes

- class GridPoint

  Grid point class (single point)
- class BaseSpatialGrid

  Base Spatial Grid class for single time step.
- class BaseDomain

  Base domain class containing multiple time steps and export methods.

5.6.1 Detailed Description

Header for Base domain class.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-03

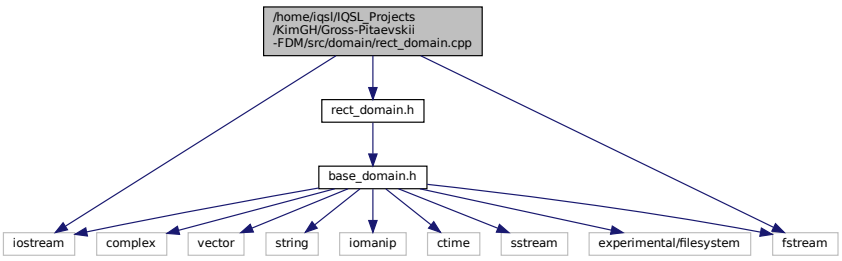
Copyright

5.7 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/domain/rect_domain.cpp File Reference

Implementation of methods in the Rectangular Domain class.

```
#include "rect_domain.h"
#include <fstream>
#include <iostream>
```

Include dependency graph for rect_domain.cpp:



5.7.1 Detailed Description

Implementation of methods in the Rectangular Domain class.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-02

Copyright

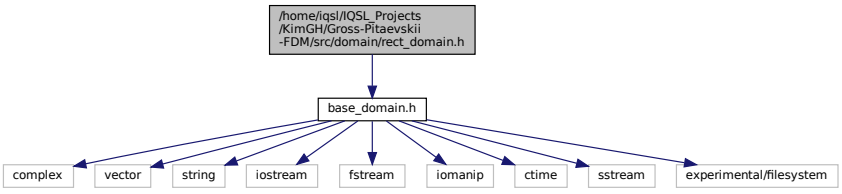
Copyright (c) 2022

5.8 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/domain/rect_domain.h File Reference

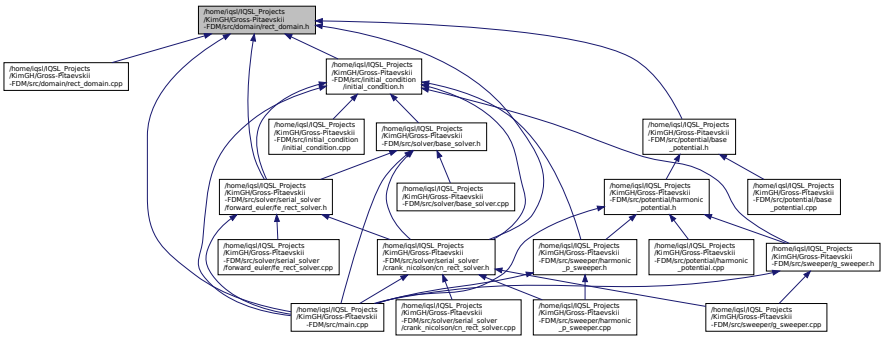
Header for Rectangular domain class.

```
#include "base_domain.h"
```

Include dependency graph for rect_domain.h:



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



Classes

- class RectangularSpatialGrid

  Rectangular Spatial Grid class for single time step.
- class RectangularDomain

  Rectangular domain containing multiple timesteps.

5.8.1 Detailed Description

Header for Rectangular domain class.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-02

Copyright

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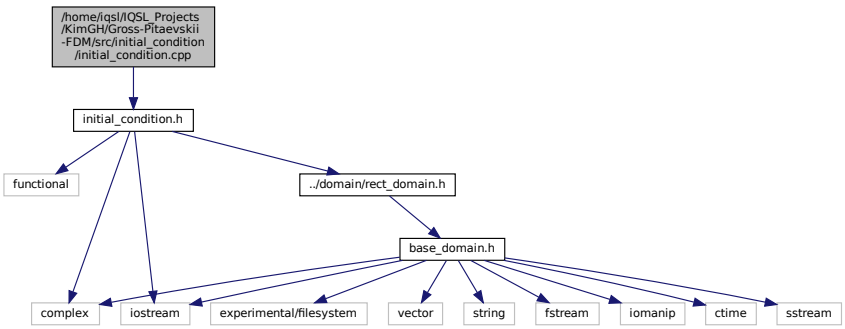
5.9 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/initial_condition/initial_condition.cpp File Reference

Implementation of initial condition class.

```
#include "initial_condition.h"
```

Include dependency graph for initial_condition.cpp:



5.9.1 Detailed Description

Implementation of initial condition class.

Author

Gyeonghun Kim, Minyoung Kim

Version

0.1

Date

2022-06-04

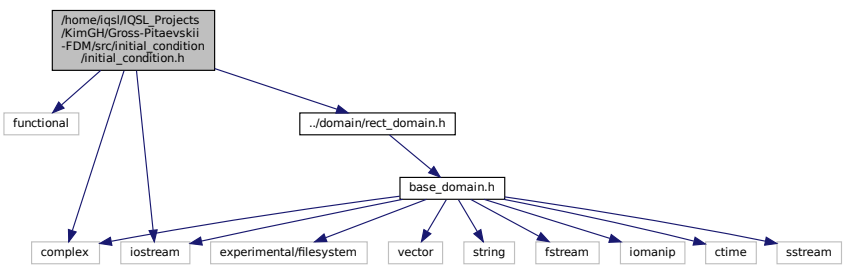
Copyright

5.10 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/initial_condition/initial_condition.h File Reference

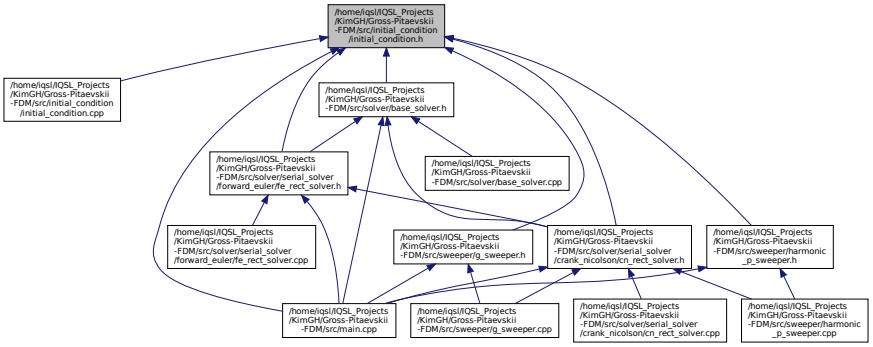
Header for the initial condition class.

```
#include <functional>
#include <complex>
#include <iostream>
#include "../domain/rect_domain.h"
```

Include dependency graph for initial_condition.h:



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



Classes

- class InitialCondition

  Initial condition class.

5.10.1 Detailed Description

Header for the initial condition class.

Author

Gyeonghun Kim, Minyoung Kim

Version

0.1

Date

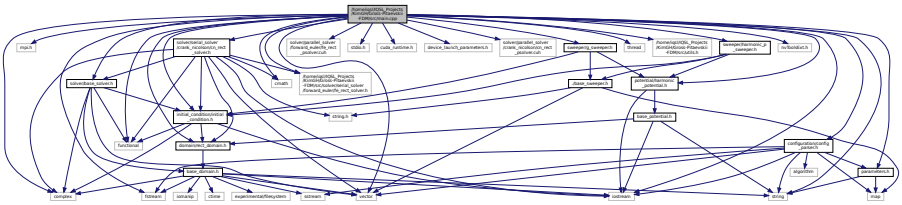
2022-06-04

Copyright

5.11 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/main.cpp File Reference

```
#include <iostream>
#include <mpi.h>
#include "domain/rect_domain.h"
#include "initial_condition/initial_condition.h"
#include "potential/harmonic_potential.h"
#include "solver/base_solver.h"
#include "solver/parallel_solver/forward_euler/fe_rect_psolver.cuh"
#include "solver/parallel_solver/crank_nicolson/cn_rect_psolver.cuh"
#include "solver/serial_solver/crank_nicolson/cn_rect_solver.h"
#include "configuration/config_parser.h"
#include "configuration/parameters.h"
#include "sweeper/g_sweeper.h"
#include "sweeper/harmonic_p_sweeper.h"
```

Include dependency graph for main.cpp:



Functions

- int main (int argc, char ∗argv[ ])

5.11.1 Function Documentation

5.11.1.1 main()

```
int main (
            int argc,
            char * argv[] )
```

Definition at line 18 of file main.cpp.

```
19 {
20     //Initialize MPI
21     MPI_Init(&argc, &argv);
22     int rank, size;
23     MPI_Comm comm = MPI_COMM_WORLD;
24     MPI_Comm_rank(comm, &rank);
25     MPI_Comm_size(comm, &size);
26     Parameters parameters;
27
28     // If argc == 1: no input configuration => use default
29     if (argc == 1)
30     {
```

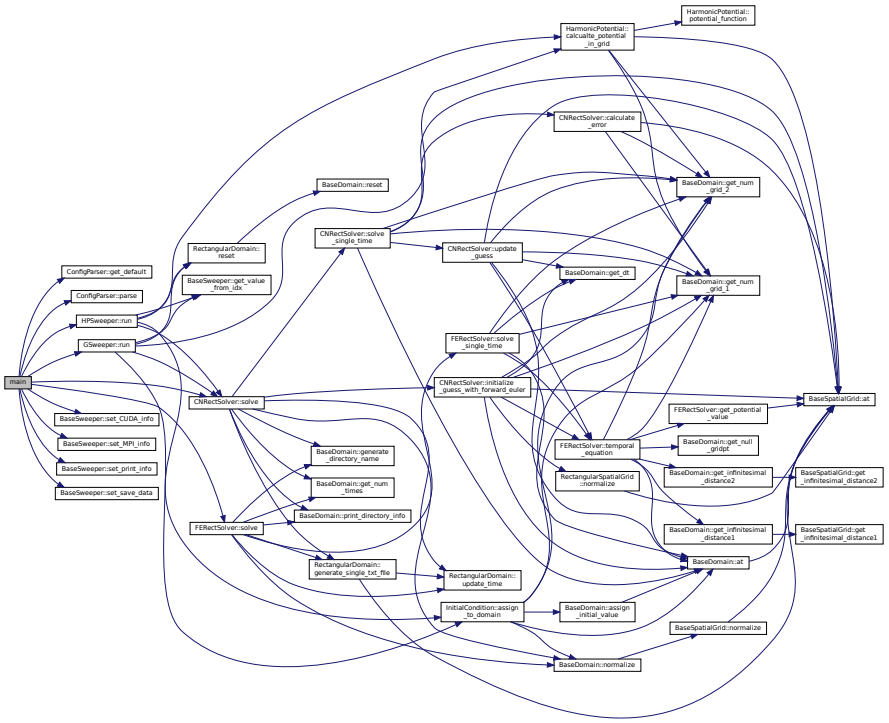
```
31          parameters = ConfigParser::get_default();
32      }
33      // argc != 1 and argc != 2 => exception
34      else if(argc != 2){
35          std::cerr « "Input config file required. " « std::endl;
36      }
37      // else: use given configuration
38      else{
39          std::string config_filename = std::string(argv[1]);
40          std::size_t dir_pos = config_filename.find_last_of("/");
41          std::string dir = config_filename.substr(0, dir_pos);
42          std::string config_name_extension = config_filename.substr(dir_pos + 1,
    config_filename.length());
43          std::string config_name = config_name_extension.substr(0, config_name_extension.length() - 4);
44
45          parameters = ConfigParser::parse(config_name, config_filename);
46      }
47
48      // Non rectangular domain is not ready in this project, but leave this part for further development
49      if (parameters.domain_parameters.domain_type == "rectangular")
50      {
51          // Single calculation
52          if (parameters.main_parameters.calculation_type == "single")
53          {
54              // Prepare domain
55              RectangularDomain *domain = new RectangularDomain(parameters.domain_parameters.n_x,
56                                                                parameters.domain_parameters.n_y,
57                                                                parameters.domain_parameters.time_start,
58                                                                parameters.domain_parameters.time_end,
59                                                                parameters.domain_parameters.n_time,
60
    parameters.domain_parameters.spatial_parameters["x_start"],
61
    parameters.domain_parameters.spatial_parameters["x_end"],
62
    parameters.domain_parameters.spatial_parameters["y_start"],
63
    parameters.domain_parameters.spatial_parameters["y_end"]);
64              // Prepare initialcondition
65              std::function<std::complex<float>(float, float)> initial_cond_function;
66              if (parameters.init_cond_parameters.init_cond_type == "singlegaussian")
67              {
68                  auto sigma_x = parameters.init_cond_parameters.init_cond_parameters["sigma_x"];
69                  auto sigma_y = parameters.init_cond_parameters.init_cond_parameters["sigma_y"];
70                  auto center_x = parameters.init_cond_parameters.init_cond_parameters["center_x"];
71                  auto center_y = parameters.init_cond_parameters.init_cond_parameters["center_y"];
72                  initial_cond_function = [center_x, center_y, sigma_x, sigma_y](float x, float y)
73                  {
74                      return std::complex<float>{
75                          float(1.) * expf(-((x - center_x) * (x - center_x) / (sigma_x * sigma_x) + (y -
    center_y) * (y - center_y) / (sigma_y * sigma_y)))
76                          };
77                  };
78                  auto *initial_condition = new InitialCondition(initial_cond_function);
79                  initial_condition->assign_to_domain(domain);
80              }
81              // Library user could add case in here if they want to use non-gaussian initial condition.
82              else
83              {
84                  std::cerr « "Unexpected initial condition" « std::endl;
85              }
86
87              // Prepare potential
88              if (parameters.equation_parameters.potential_type == "harmonic")
89              {
90                  auto omega_x = parameters.equation_parameters.potential_parameters["omega_x"];
91                  auto omega_y = parameters.equation_parameters.potential_parameters["omega_y"];
92                  auto *potential = new HarmonicPotential(omega_x, omega_y);
93                  potential->calcualte_potential_in_grid(domain);
94              }
95              // Library user could add case in here if they want to use non-harmonic potential
96              else
97              {
98                  std::cerr « "Unexpected initial condition" « std::endl;
99              }
100
101             float g = parameters.equation_parameters.g;
102
103             bool save_data = parameters.solver_parameters.save_data;
104             bool print_info = parameters.solver_parameters.print_info;
105
106             // Solve equation in given method from configuration
107             if (parameters.solver_parameters.method == "cranknicolson")
108             {
109                 if(parameters.solver_parameters.run_parallel){
110                     float converge_crit =
    parameters.solver_parameters.solver_parameters["converge_crit"];
```

```
111                     int max_iter = parameters.solver_parameters.int_parameters["max_iter"];
112                     int cuda_device = parameters.solver_parameters.int_parameters["cuda_device"];
113                     CNRectPSolver solver = CNRectPSolver(g, domain, cuda_device);
114                     solver.solve(converge_crit, max_iter, std::to_string(rank), print_info, save_data);
115                 }
116                 else{
117                     float converge_crit =
    parameters.solver_parameters.solver_parameters["converge_crit"];
118                     int max_iter = parameters.solver_parameters.int_parameters["max_iter"];
119                     CNRectSolver solver = CNRectSolver(g, domain);
120                     //std::cout<<"save_data " <<save_data<<std::endl;
121                     solver.solve(converge_crit, max_iter, std::to_string(rank), print_info, save_data);
122                 }
123             }
124             else if (parameters.solver_parameters.method == "forwardeuler"){
125                 if (parameters.solver_parameters.run_parallel)
126                 {
127                     int cuda_device = parameters.solver_parameters.int_parameters["cuda_device"];
128                     FERectPSolver solver = FERectPSolver(g, domain, cuda_device);
129                     solver.solve(std::to_string(rank), print_info, save_data);
130                 }
131                 else
132                 {
133                     FERectSolver solver = FERectSolver(g, domain);
134                     solver.solve(std::to_string(rank), print_info, save_data);
135                 }
136             }
137         }
138         else if (parameters.main_parameters.calculation_type == "g_sweep")
139         {
140             // Prepare G sweep
141             GSweeper gSweeper = GSweeper(parameters.main_parameters.float_parameters["sweep_start"],
142                                          parameters.main_parameters.float_parameters["sweep_end"],
143                                          parameters.main_parameters.int_parameters["sweep_count"],
144                                          bool(parameters.main_parameters.int_parameters["end_point"]));
145             // Initialze domain
146             RectangularDomain *domain = new RectangularDomain(parameters.domain_parameters.n_x,
147                                                               parameters.domain_parameters.n_y,
148                                                               parameters.domain_parameters.time_start,
149                                                               parameters.domain_parameters.time_end,
150                                                               parameters.domain_parameters.n_time,
151
    parameters.domain_parameters.spatial_parameters["x_start"],
152
    parameters.domain_parameters.spatial_parameters["x_end"],
153
    parameters.domain_parameters.spatial_parameters["y_start"],
154
    parameters.domain_parameters.spatial_parameters["y_end"]);
155
156             // Prepare initial condition
157             std::function<std::complex<float>(float, float)> initial_cond_function;
158             if (parameters.init_cond_parameters.init_cond_type == "singlegaussian")
159             {
160                 // prepare initial condition
161                 auto sigma_x = parameters.init_cond_parameters.init_cond_parameters["sigma_x"];
162                 auto sigma_y = parameters.init_cond_parameters.init_cond_parameters["sigma_y"];
163                 auto center_x = parameters.init_cond_parameters.init_cond_parameters["center_x"];
164                 auto center_y = parameters.init_cond_parameters.init_cond_parameters["center_y"];
165                 initial_cond_function = [center_x, center_y, sigma_x, sigma_y](float x, float y)
166                 {
167                     return std::complex<float>{
168                         float(1.) * expf(-((x - center_x) * (x - center_x) / (sigma_x * sigma_x) + (y -
    center_y) * (y - center_y) / (sigma_y * sigma_y)))};
169                 };
170                 auto *initial_condition = new InitialCondition(initial_cond_function);
171                 initial_condition->assign_to_domain(domain);
172
173                 // Prepare potential
174                 if (parameters.equation_parameters.potential_type == "harmonic")
175                 {
176                     auto omega_x = parameters.equation_parameters.potential_parameters["omega_x"];
177                     auto omega_y = parameters.equation_parameters.potential_parameters["omega_y"];
178                     auto *potential = new HarmonicPotential(omega_x, omega_y);
179                     potential->calcualte_potential_in_grid(domain);
180
181                     bool save_data = parameters.solver_parameters.save_data;
182                     bool print_info = parameters.solver_parameters.print_info;
183                     bool cuda_use = (bool)parameters.main_parameters.int_parameters["cuda_use"];
184                     bool mpi_use = (bool)parameters.main_parameters.int_parameters["mpi_use"];
185                     if (cuda_use)
186                     {
187                         // setup cuda if cuda_use
188                         gSweeper.set_CUDA_info(parameters.main_parameters.int_parameters["gpu_count"],
189
    parameters.main_parameters.int_parameters["calculation_per_gpu"]);
190                     }
```

```
191                     if (mpi_use)
192                     {
193                         // setup MPI if mpi_use
194                         gSweeper.set_MPI_info(rank, size);
195                     }
196                     // Setup whether print through standard output or not
197                     gSweeper.set_print_info(print_info);
198                     // Setup whether save data or not
199                     gSweeper.set_save_data(save_data);
200                     // Run sweeping
201                     gSweeper.run(domain, initial_condition, potential);
202                 }
203                 else
204                 {
205                     std::cerr « "Unexpected initial condition" « std::endl;
206                 }
207             }
208             else
209             {
210                 std::cerr « "Unexpected initial condition" « std::endl;
211             }
212         }
213         else if (parameters.main_parameters.calculation_type == "anisotropy_sweep")
214         {
215             // Prepare Harmonic Potential Sweeper
216             HPSweeper hpSweeper = HPSweeper(parameters.main_parameters.float_parameters["sweep_start"],
217                                             parameters.main_parameters.float_parameters["sweep_end"],
218                                             parameters.main_parameters.int_parameters["sweep_count"],
219 
    bool(parameters.main_parameters.int_parameters["end_point"]));
220             // Prepare domain
221             RectangularDomain *domain = new RectangularDomain(parameters.domain_parameters.n_x,
222                                                               parameters.domain_parameters.n_y,
223                                                               parameters.domain_parameters.time_start,
224                                                               parameters.domain_parameters.time_end,
225                                                               parameters.domain_parameters.n_time,
226 
    parameters.domain_parameters.spatial_parameters["x_start"],
227 
    parameters.domain_parameters.spatial_parameters["x_end"],
228 
    parameters.domain_parameters.spatial_parameters["y_start"],
229 
    parameters.domain_parameters.spatial_parameters["y_end"]);
230             // Prepare initial Condition
231             std::function<std::complex<float>(float, float)> initial_cond_function;
232             if (parameters.init_cond_parameters.init_cond_type == "singlegaussian")
233             {
234                 // Prepare initial condition
235                 auto sigma_x = parameters.init_cond_parameters.init_cond_parameters["sigma_x"];
236                 auto sigma_y = parameters.init_cond_parameters.init_cond_parameters["sigma_y"];
237                 auto center_x = parameters.init_cond_parameters.init_cond_parameters["center_x"];
238                 auto center_y = parameters.init_cond_parameters.init_cond_parameters["center_y"];
239                 initial_cond_function = [center_x, center_y, sigma_x, sigma_y](float x, float y)
240                 {
241                     return std::complex<float>{
242                         float(1.) * expf(-((x - center_x) * (x - center_x) / (sigma_x * sigma_x) + (y -
    center_y) * (y - center_y) / (sigma_y * sigma_y)))};
243                 };
244                 auto *initial_condition = new InitialCondition(initial_cond_function);
245                 initial_condition->assign_to_domain(domain);
246 
247                 if (parameters.equation_parameters.potential_type == "harmonic")
248                 {
249                     // setup save / MPI use / cuda use / print option
250                     float g = parameters.equation_parameters.g;
251                     bool save_data = parameters.solver_parameters.save_data;
252                     bool print_info = parameters.solver_parameters.print_info;
253                     bool cuda_use = (bool)parameters.main_parameters.int_parameters["cuda_use"];
254                     bool mpi_use = (bool)parameters.main_parameters.int_parameters["mpi_use"];
255                     if (cuda_use)
256                     {
257                         hpSweeper.set_CUDA_info(parameters.main_parameters.int_parameters["gpu_count"],
258 
    parameters.main_parameters.int_parameters["calculation_per_gpu"]);
259                     }
260                     if (mpi_use)
261                     {
262                         hpSweeper.set_MPI_info(rank, size);
263                     }
264                     hpSweeper.set_print_info(print_info);
265                     hpSweeper.set_save_data(save_data);
266 
267                     hpSweeper.run(domain, initial_condition, g);
268                 }
269                 else
270                 {
```

```
271                     std::cerr « "Unexpected initial condition" « std::endl;
272                 }
273             }
274             else
275             {
276                 std::cerr « "Unexpected initial condition" « std::endl;
277             }
278         }
279     }
280     else
281     {
282         std::cerr « "Unexpected Domain" « std::endl;
283     }
284     // Finialize MPI
285     MPI_Finalize();
286 }
```

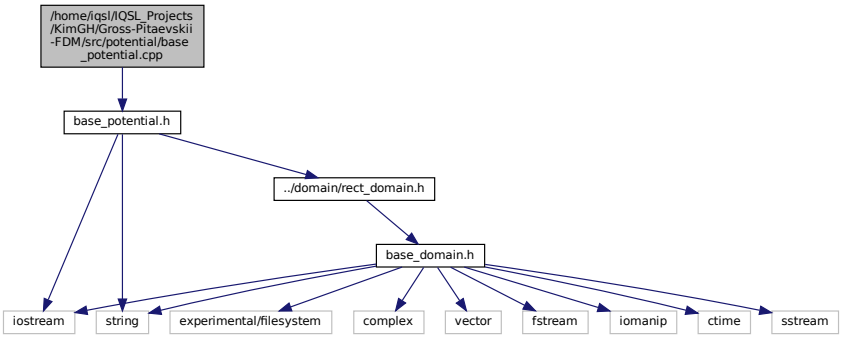
Here is the call graph for this function:



5.12 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/potential/base_potential.cpp File Reference

Implementation of the methods in potential class.

```
#include "base_potential.h"
```
Include dependency graph for base_potential.cpp:



5.12.1 Detailed Description

Implementation of the methods in potential class.

Author

Gyeonghun Kim, Minyoung Kim

Version

0.1

Date

2022-06-08

Copyright

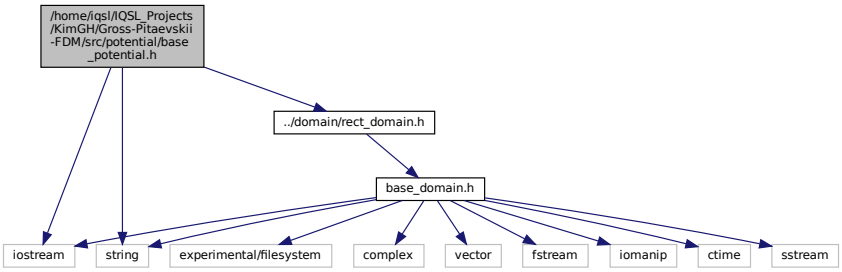
5.13 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/potential/base_potential.h File Reference

Header for the base potential class. Heritate this class for create custom potential shape.

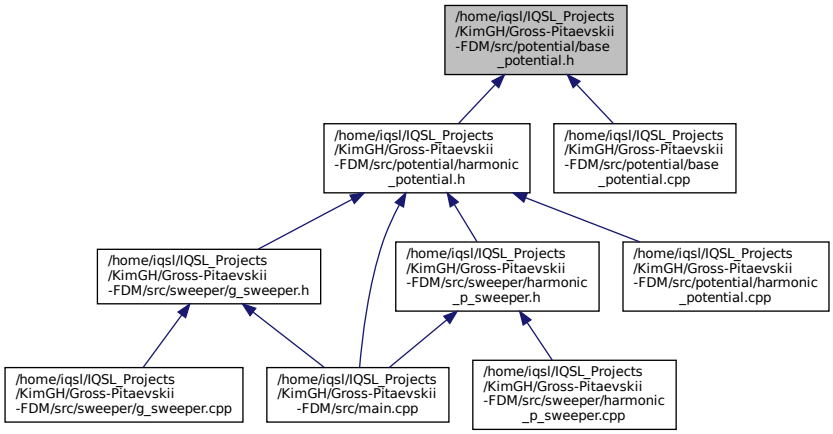
```
#include <iostream>
#include <string>
```

```
#include "../domain/rect_domain.h"
```

Include dependency graph for base_potential.h:



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



Classes

- class BasePotential

5.13.1 Detailed Description

Header for the base potential class. Heritate this class for create custom potential shape.

Author

Gyeonghun Kim, Minyoung Kim

Version

0.1

Date

2022-06-08

Copyright

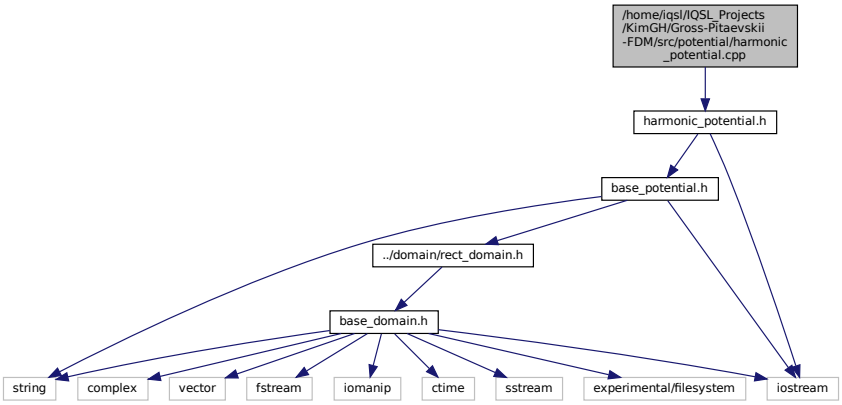
Copyright (c) 2022

5.14 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/potential/harmonic_potential.cpp File Reference

Implementation of harmonic potential methods.

```
#include "harmonic_potential.h"
```

Include dependency graph for harmonic_potential.cpp:



5.14.1 Detailed Description

Implementation of harmonic potential methods.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-08

Copyright

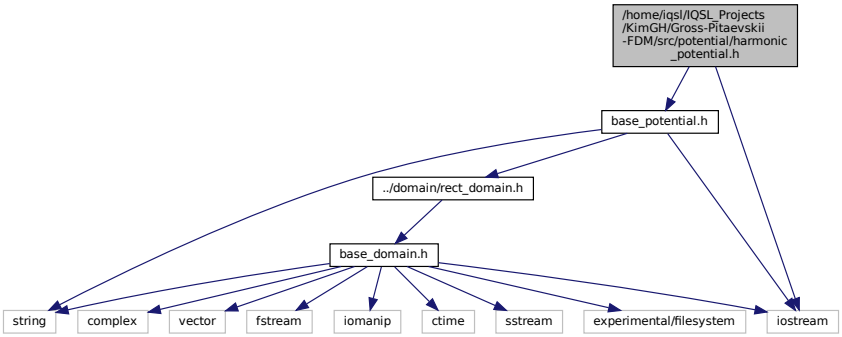
Copyright (c) 2022

5.15 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/potential/harmonic_potential.h File Reference

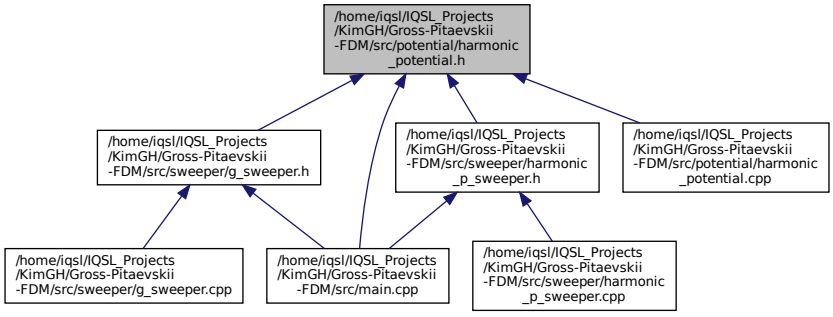
Header file for harmoni potential (V = 0.5 ∗ (omega_x^2 ∗ x^2 + omega_y^2 ∗ y^2)

```
#include <iostream>
#include "base_potential.h"
```

Include dependency graph for harmonic_potential.h:



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



Classes

- class HarmonicPotential

5.15.1 Detailed Description

Header file for harmoni potential (V = 0.5 ∗ (omega_x^2 ∗ x^2 + omega_y^2 ∗ y^2)

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-08

Copyright

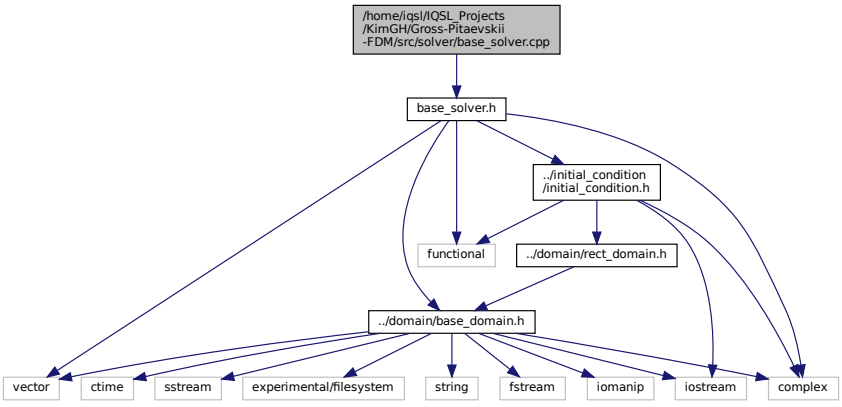
Copyright (c) 2022

5.16 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/solver/base_solver.cpp File Reference

Header file for base solver.

```
#include "base_solver.h"
```

Include dependency graph for base_solver.cpp:



5.16.1 Detailed Description

Header file for base solver.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-05

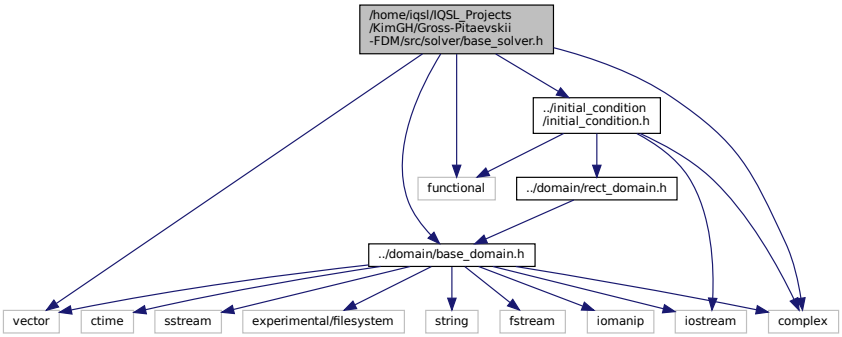
Copyright

5.17 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/solver/base_solver.h File Reference

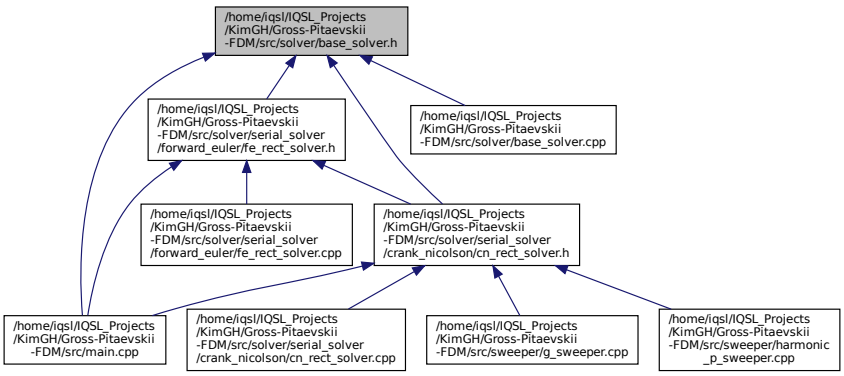
Implementation file for base solver.

```
#include <complex>
#include <vector>
#include <functional>
#include "../domain/base_domain.h"
#include "../initial_condition/initial_condition.h"
```

Include dependency graph for base_solver.h:



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



Classes

- class BaseSolver

  Base Solver for Gross Piteavskill finite difference solver.

5.17.1 Detailed Description

Implementation file for base solver.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-05

Copyright

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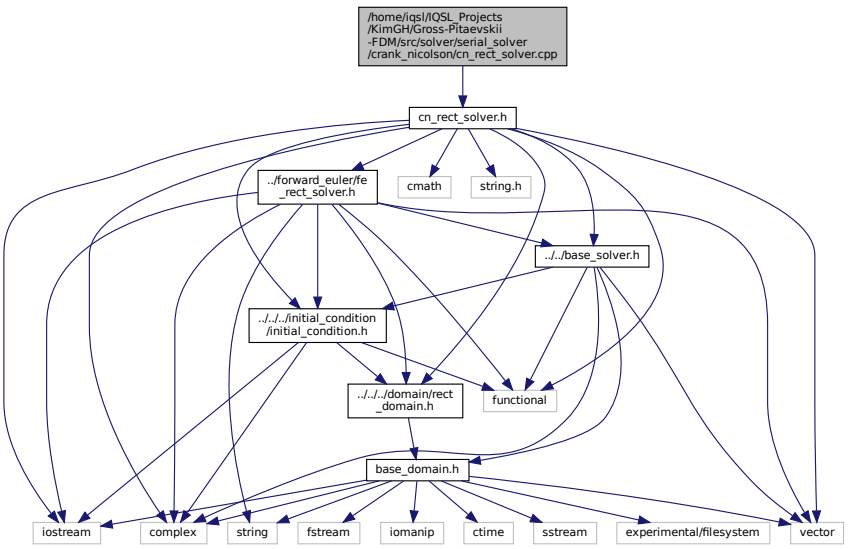
5.18 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/solver/serial_solver/crank_nicolson/cn_rect_solver.cpp File Reference

Implementation file for serial crank nicolson solver.

```
#include "cn_rect_solver.h"
```

Include dependency graph for cn_rect_solver.cpp:



5.18.1 Detailed Description

Implementation file for serial crank nicolson solver.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-05

Copyright

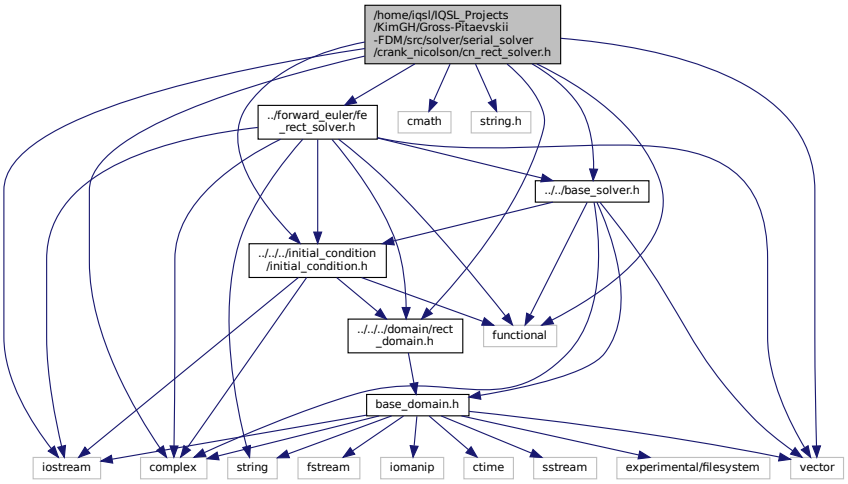
Copyright (c) 2022

5.19 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/solver/serial_solver/crank_nicolson/cn_rect_solver.h File Reference

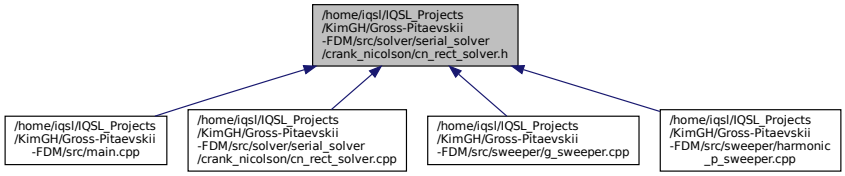
Header file for serial crank nicolson solver.

```
#include <complex>
#include <vector>
#include <functional>
#include <iostream>
#include <cmath>
#include <string.h>
#include "../../../domain/rect_domain.h"
#include "../../../initial_condition/initial_condition.h"
#include "../../base_solver.h"
#include "../forward_euler/fe_rect_solver.h"
```

Include dependency graph for cn_rect_solver.h:



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



Classes

- class CNRectSolver

5.19.1 Detailed Description

Header file for serial crank nicolson solver.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-05

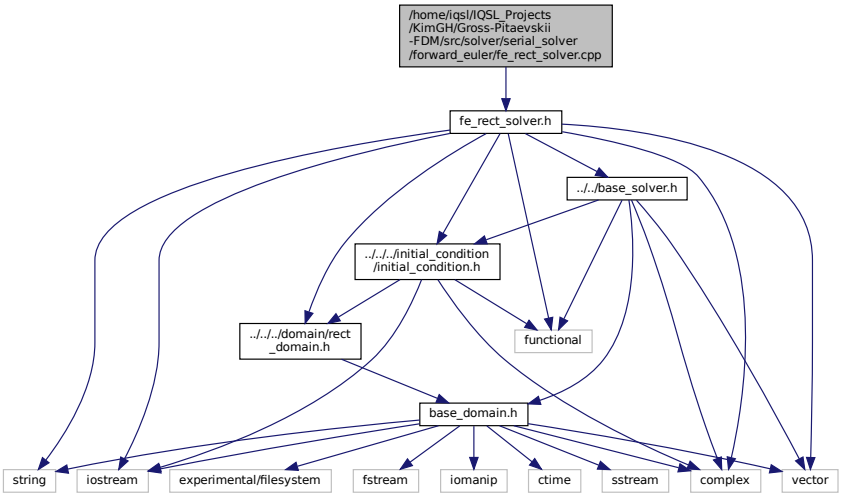
Copyright

5.20 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/solver/serial_solver/forward_euler/fe_rect_solver.cpp File Reference

Implementation file for serial forward euler solver methods.

```
#include "fe_rect_solver.h"
```

Include dependency graph for fe_rect_solver.cpp:



5.20.1 Detailed Description

Implementation file for serial forward euler solver methods.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-05

Copyright

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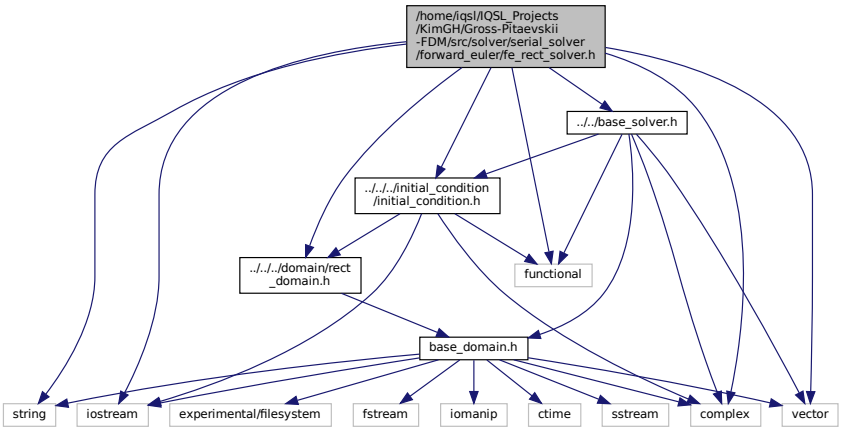
5.21 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/solver/serial_solver/forward_euler/fe_rect_solver.h File Reference

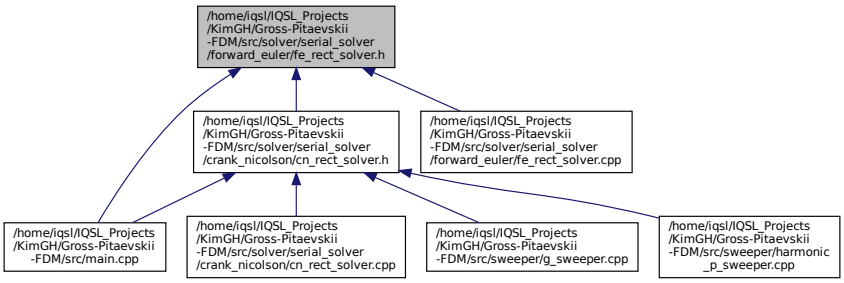
Header file for serial forward euler solver.

```
#include <complex>
#include <vector>
#include <functional>
#include <iostream>
#include <string>
#include "../../../domain/rect_domain.h"
#include "../../../initial_condition/initial_condition.h"
#include "../../base_solver.h"
```

Include dependency graph for fe_rect_solver.h:



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



Classes

- class FERectSolver

  Forward Euler Serial Solver.

5.21.1 Detailed Description

Header file for serial forward euler solver.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

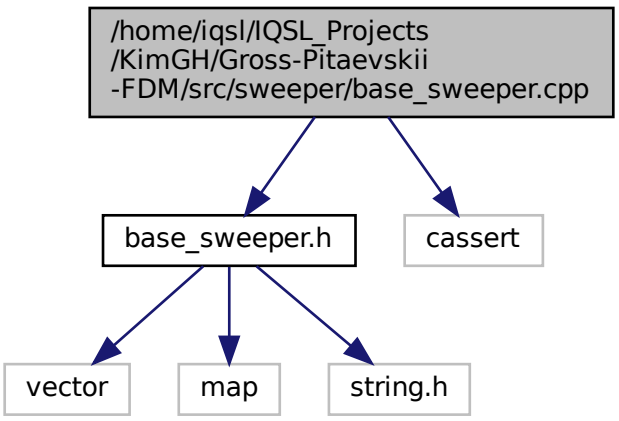
2022-06-05

Copyright

5.22 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/sweeper/base_sweeper.cpp File Reference

```
#include "base_sweeper.h"
#include <cassert>
```

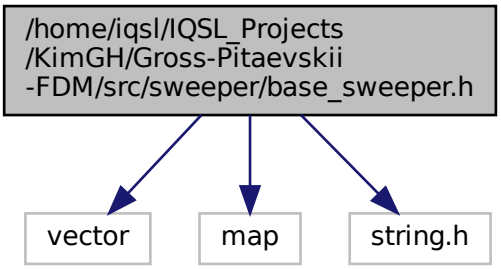
Include dependency graph for base_sweeper.cpp:



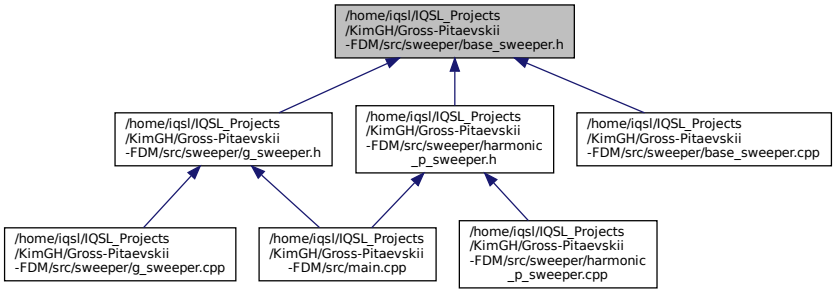
5.23 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/sweeper/base_sweeper.h File Reference

```
#include <vector>
#include <map>
#include <string.h>
```

Include dependency graph for base_sweeper.h:



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



Classes

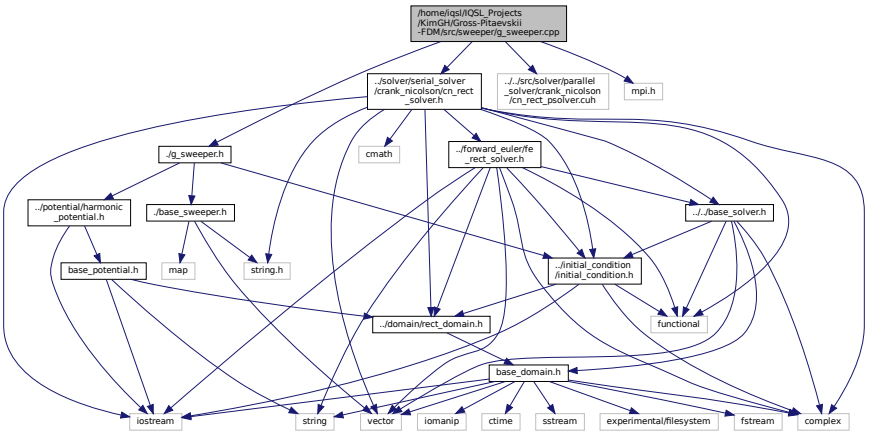
- class BaseSweeper

5.24 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/sweeper/g_sweeper.cpp File Reference

```
#include "./g_sweeper.h"
#include "../solver/serial_solver/crank_nicolson/cn_rect_solver.h"
```

```
#include "../../src/solver/parallel_solver/crank_nicolson/cn_rect_psolver.↩
cuh"
#include <mpi.h>
```

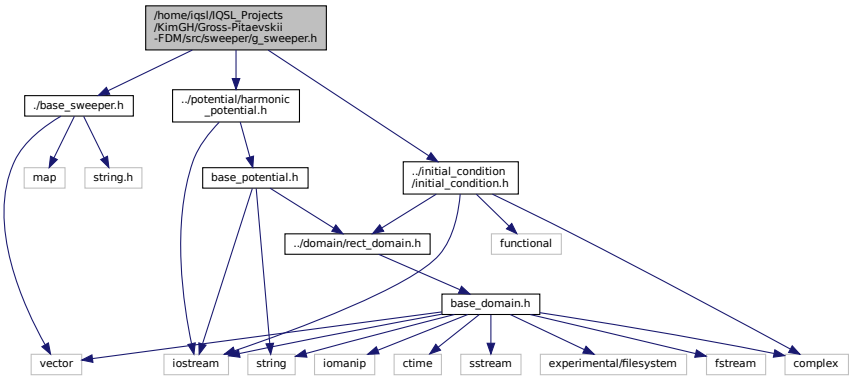
Include dependency graph for g_sweeper.cpp:



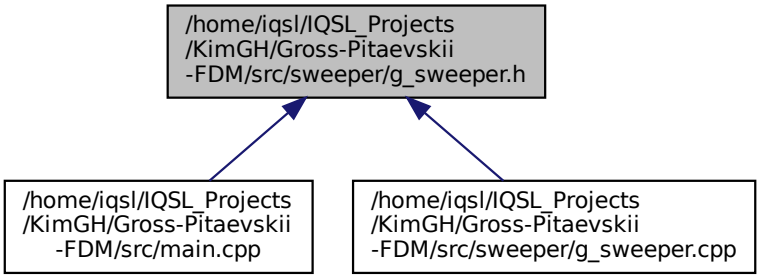
5.25 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/sweeper/g_sweeper.h File Reference

```
#include "./base_sweeper.h"
#include "../potential/harmonic_potential.h"
#include "../initial_condition/initial_condition.h"
```

Include dependency graph for g_sweeper.h:



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



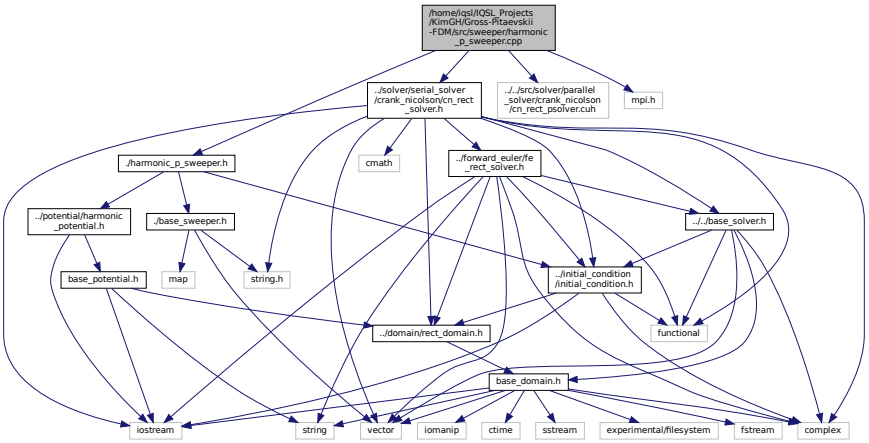
Classes

- class GSweeper

5.26 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/sweeper/harmonic_p_sweeper.cpp File Reference

```
#include "./harmonic_p_sweeper.h"
#include "../solver/serial_solver/crank_nicolson/cn_rect_solver.h"
#include "../../src/solver/parallel_solver/crank_nicolson/cn_rect_psolver.↩
cuh"
#include <mpi.h>
```

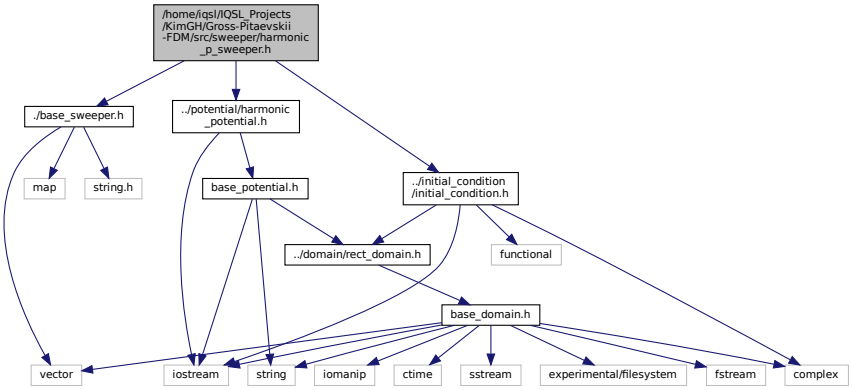
Include dependency graph for harmonic_p_sweeper.cpp:



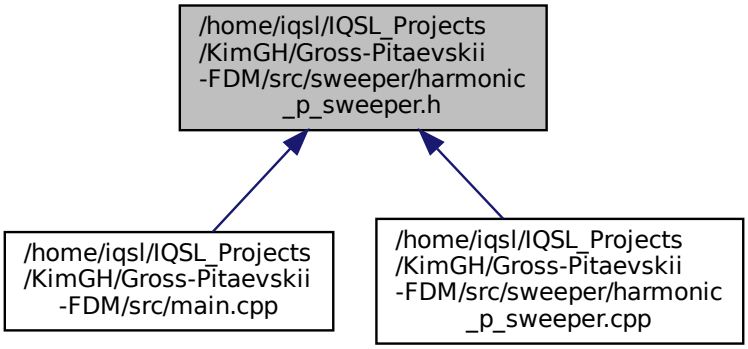
5.27 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD↩ M/src/sweeper/harmonic_p_sweeper.h File Reference

```
#include "./base_sweeper.h"
#include "../potential/harmonic_potential.h"
#include "../initial_condition/initial_condition.h"
```

Include dependency graph for harmonic_p_sweeper.h:



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



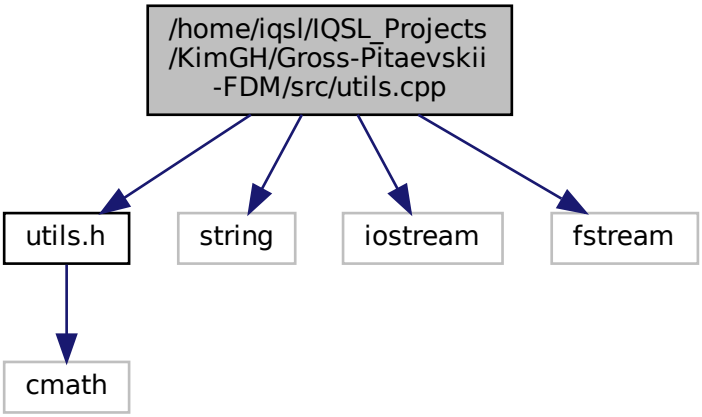
Classes

- class HPSweeper

5.28 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/utils.cpp File Reference

```
#include "utils.h"
#include <string>
#include <iostream>
#include <fstream>
```

Include dependency graph for utils.cpp:



Functions

- bool is_close (float a, float b, float tolerance)

5.28.1 Function Documentation

5.28.1.1 is_close()

```
bool is_close (
            float a,
            float b,
            float tolerance )
```

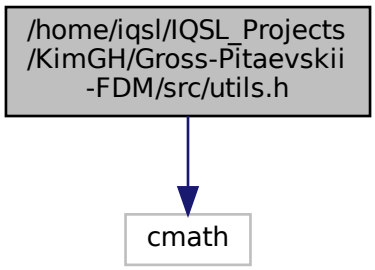
Definition at line 5 of file utils.cpp.

```
5                                           {
6     return std::abs(a - b) < tolerance;
7 }
```

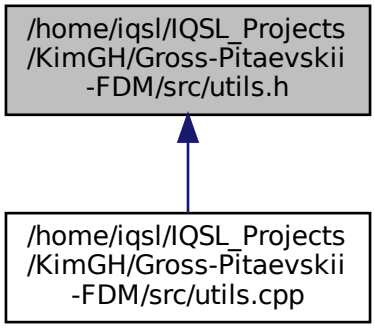
5.29 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/utils.h File Reference

```
#include <cmath>
```

Include dependency graph for utils.h:



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



Functions

- bool is_close (float a, float b, float tolerance)

5.29.1 Function Documentation

5.29.1.1 is_close()

```
bool is_close (
              float a,
              float b,
              float tolerance )
```

Definition at line 5 of file utils.cpp.

```
5                                                {
6     return std::abs(a - b) < tolerance;
7 }
```

Index