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:

BaseDomain
RectangularDomain
BasePotential
HarmonicPotential
BaseSolver
FERectSolver
CNRectSolver
BaseSpatialGrid
RectangularSpatialGrid
BaseSweeper
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2 Hierarchical Index

Chapter 2

Class Index

2.1 Class List

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

BaseDomain
Base domain class containing multiple time steps and export methods
BasePotential
BaseSolver
Base Solver for Gross Piteavskill finite difference solver
BaseSpatialGrid
Base Spatial Grid class for single time step
BaseSweeper
CNRectSolver
ConfigParser
Configuration parser
DomainParameters
Domain branch parameters containing information about domain
EquationParameters
Equation branch parameters containing information about equation
FERectSolver
Forward Euler Serial Solver
GridPoint
Grid point class (single point)
GSweeper
HarmonicPotential
HPSweeper
InitialCondition
Initial condition class
InitialConditionParameters
Initial condition branch parameters containing information about initial condition
MainParameters
Main branch parameters containing information about overall calculation
Parameters
Parameters containing configuration name and all other branched parameters
RectangularDomain
Rectangular domain containing multiple timesteps
RectangularSpatialGrid
Rectangular Spatial Grid class for single time step
SolverParameters
Solver branch parameters containing information about solver

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Chapter 3

File Index

3.1 File List

Here is a list of all files with brief descriptions:

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Chapter 4

Class Documentation

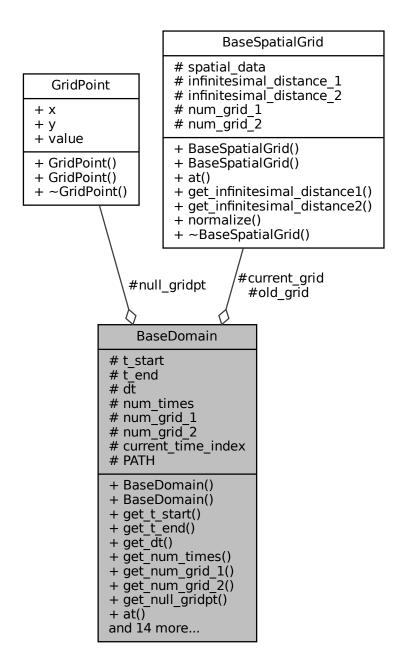
4.1 BaseDomain Class Reference

Base domain class containing multiple time steps and export methods.

Inheritance diagram for BaseDomain:

BaseDomain # old_grid # current_grid # null_gridpt # t_start # t_end # dt # num_times # num_grid_1 # num_grid_2 # current_time_index # PATH + BaseDomain() + BaseDomain() + get_t_start() + get_t_end() + get_dt() + get_num_times() + get_num_grid_1() + get_num_grid_2() + get_null_gridpt() + at() and 14 more... RectangularDomain + potential_grid - x_start - x_end - y_start y_end + RectangularDomain() + RectangularDomain() + get_x_start() + get_x_start() + get_y_start() + get_x_end() + get_y_end() + generate_single_txt_file() + update_time() + reset() + ~RectangularDomain()

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.

```
this->t_start = t_start;
this->t_end = t_end;
this->num_times = num_times;

// dt: interval of time
this->dt = (t_end - t_start) / (num_times - 1);
this->num_grid_1 = num_grid_1;
this->num_grid_2 = num_grid_2;
this->old_grid = new BaseSpatialGrid(num_grid_1, num_grid_2);
this->current_grid = new BaseSpatialGrid(num_grid_1, num_grid_2);
this->null_gridpt = new GridPoint(0, 0, std::complex<float>{0});
```

4.1.2.3 ∼BaseDomain()

```
BaseDomain::\simBaseDomain ( )
```

Definition at line 100 of file base_domain.cpp.

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⊷	$x = x_start + index_1*dx$
_1	
index⊷	y = y_start + index_2 * dy
_2	
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.

Here is the call graph for this function:



4.1.3.3 at()

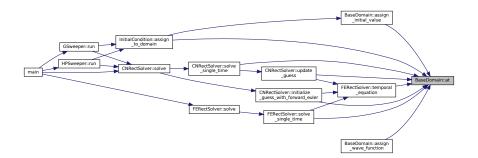
Definition at line 153 of file base_domain.cpp.

```
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
            return this->old_grid->at(index_1, index_2);
161
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()

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

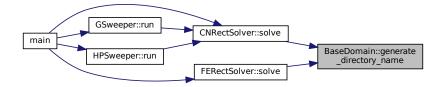
Returns

std::string directory name with "/"

Definition at line 203 of file base_domain.cpp.

```
205
        auto t = std::time(nullptr);
206
207
        auto tm = *std::localtime(&t);
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;
        // else if(print_info )
217
218
        //TODO
        else if (!created)
219
220
221
            std::cout « "Creating directory failed" « std::endl;
223
        this->PATH = directory_name + "/";
224
225 }
```

Here is the caller graph for this function:



4.1.3.5 generate_single_txt_file()

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

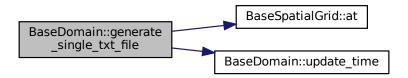
Parameters

grid	grid at t
filename	file name to store data

Definition at line 235 of file base_domain.cpp.

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

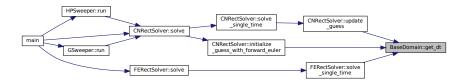
4.1.3.7 get_dt()

```
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()

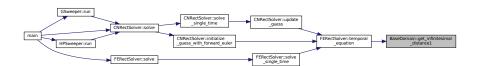
```
float BaseDomain::get_infinitesimal_distance1 ( )
```

Definition at line 143 of file base_domain.cpp.

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 ( )
```

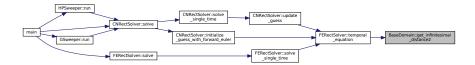
Definition at line 147 of file base_domain.cpp.

```
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:



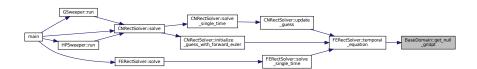
4.1.3.10 get_null_gridpt()

```
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:



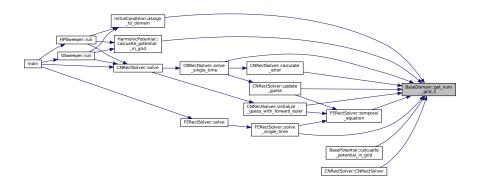
4.1.3.11 get_num_grid_1()

```
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:



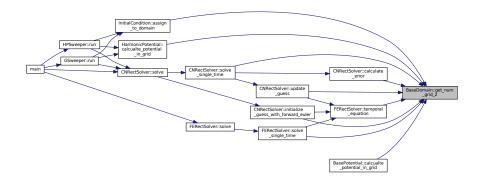
4.1.3.12 get_num_grid_2()

```
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:

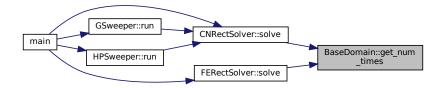


4.1.3.13 get_num_times()

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

Definition at line 129 of file base_domain.cpp.

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()

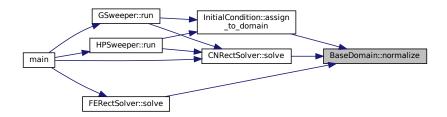
Definition at line 111 of file base_domain.cpp.

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

Here is the call graph for this function:



Here is the caller graph for this function:



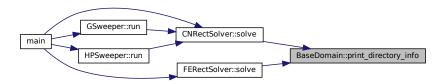
4.1.3.18 print_directory_info()

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

Definition at line 261 of file base_domain.cpp. $^{262}\ \ \{$

```
std::cout « this->num_times;
std::cout « " text files are generated in \n";
std::cout « this->PATH « std::endl;
std::cout « this->PATH »
```

Here is the caller graph for this function:



4.1.3.19 reset()

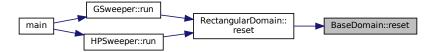
```
void BaseDomain::reset ( ) [virtual]
```

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()

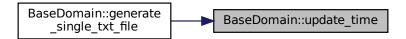
4.1.3.21 update_time()

```
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);
              this->old_grid = this->current_grid;
this->current_grid = new BaseSpatialGrid(num_grid_1, num_grid_2);
277
278
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.

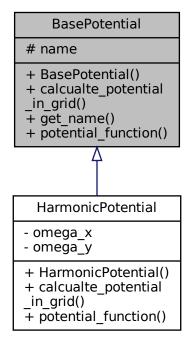
The documentation for this class was generated from the following files:

- /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:

BasePotential
name
+ BasePotential() + calcualte_potential _in_grid() + get_name() + potential_function()

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()

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.

```
int num_grid_1 = domain->get_num_grid_1();
int num_grid_2 = domain->get_num_grid_2();
```

```
for (auto i = 0; i < num_grid_1; ++i)

{
    for (auto j = 0; j < num_grid_2; ++j)

    {
        auto point = domain->potential_grid->at(i, j);

        //Assign potential value in potential grid
        point->value = std::complex<float>{this->potential_function(point->x, point->y), 0};

}

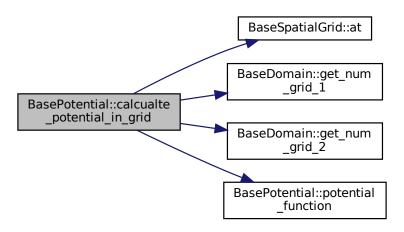
}

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 (  \label{eq:float x, float x, float y} float y )
```

Default potental function for constant zero potential.

Parameters

Χ	
У	

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:

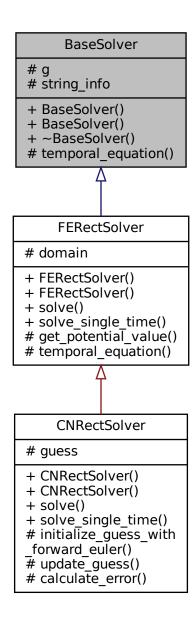
- /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/potential/base_potential.h
- $\bullet \ / home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/potential/base_potential.cpp$

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:

g # string_info + BaseSolver() + BaseSolver() + ~BaseSolver() # temporal_equation()

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 ( {\tt float} \  \, {\tt g\_} \  \, )
```

Construct a new Base Solver:: Base Solver object.

Parameters

```
g←
_←
```

Definition at line 18 of file base_solver.cpp.

4.3.2.3 \sim BaseSolver()

```
BaseSolver::\simBaseSolver ( )
```

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()

defualt temporal equation

Returns

```
std::complex<float> 0+0i
```

Definition at line 36 of file base_solver.cpp.

```
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:

BaseSpatialGrid # spatial data # infinitesimal_distance_1 # infinitesimal_distance_2 # num_grid_1 # num_grid_2 + BaseSpatialGrid() + BaseSpatialGrid() + get_infinitesimal_distance1() + get_infinitesimal_distance2() + normalize() + ~BaseSpatialGrid() RectangularSpatialGrid - x start x_end - y_start y_end + RectangularSpatialGrid() + RectangularSpatialGrid() + ~RectangularSpatialGrid() + normalize()

Collaboration diagram for BaseSpatialGrid:

spatial_data # infinitesimal_distance_1 # infinitesimal_distance_2 # num_grid_1 # num_grid_2 + BaseSpatialGrid() + BaseSpatialGrid() + at() + get_infinitesimal_distance1() + get_infinitesimal_distance2() + normalize() + ~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.

```
18
        this->num_grid_1 = num_grid_1;
       this->num_grid_2 = num_grid_2;
19
        //Spatial_data: 2D matrix of grid points
       this->spatial_data = std::vector<std::vector<GridPoint»(num_grid_1);
for (auto i = 0; i < num_grid_1; ++i)
21
22
2.3
24
            this->spatial_data[i] = std::vector<GridPoint>(num_grid_2);
26
        this-> infinitesimal_distance_1 = 1.f;
27
        this -> infinitesimal_distance_2 = 1.f;
28 }
```

4.4.2.3 \sim BaseSpatialGrid()

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

Definition at line 51 of file base_domain.cpp.

```
for (auto i = 0; i < num_grid_1; ++i)

for (auto i = 0; i < num_grid_1; ++i)

this->spatial_data[i].clear();

std::vector<GridPoint>().swap(this->spatial_data[i]);

this->spatial_data.clear();

std::vector<std::vector<GridPoint*().swap(this->spatial_data);

this->spatial_data.clear();

std::vector<std::vector<GridPoint*().swap(this->spatial_data);
```

4.4.3 Member Function Documentation

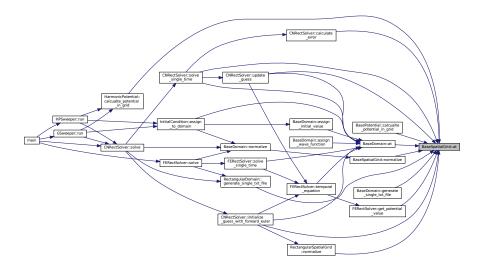
4.4.3.1 at()

```
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()

```
{\tt 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.

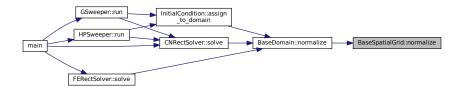
```
31 {
32
33
        for (auto i = 0; i < this->num_grid_1; ++i)
34
35
            for (auto j = 0; j < this->num_grid_2; ++j)
36
37
                 auto wave_func = this->at(i, j)->value;
                 sum += float(std::pow(std::abs(wave_func), 2));
38
39
40
        sum = std::sqrt(sum * this->infinitesimal_distance_1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

Here is the call graph for this function:

```
BaseSpatialGrid::at

BaseSpatialGrid::at
```

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

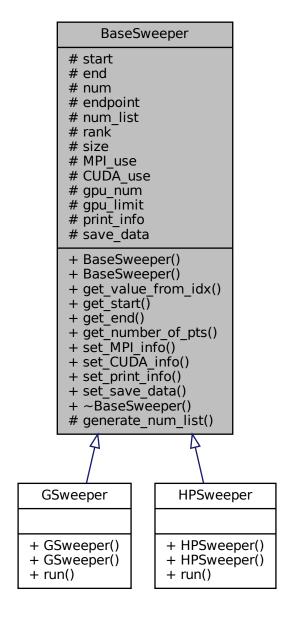
int BaseSpatialGrid::num_grid_2 [protected]

Definition at line 60 of file base_domain.h.

38 **Class Documentation** 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

Inheritance diagram for BaseSweeper:



Collaboration diagram for BaseSweeper:

```
BaseSweeper
# start
# end
# num
# endpoint
# num list
# rank
# size
# MPI use
# CUDA_use
# gpu_num
# gpu limit
# print_info
# save_data
+ BaseSweeper()
+ BaseSweeper()
+ get_value_from_idx()
+ get_start()
+ get end()
+ get_number_of_pts()
+ set_MPI_info()
+ set_CUDA_info()
+ set_print_info()
+ set save data()
+ ~BaseSweeper()
# generate num list()
```

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
- $\bullet \ \ \mathsf{vector} \! < \mathsf{float} > \! \mathsf{num_list}$
- 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.

```
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 \sim BaseSweeper()

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

Definition at line 63 of file base_sweeper.cpp.

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);
float d = 0.;
17
         if(this->endpoint){
18
19
             d = (this \rightarrow end - this \rightarrow start) / float(this \rightarrow num -1);
         }else{
21
              d = (this -> end - this-> start ) / float(this-> num);
22
2.3
         for (int i=0; i<this -> num; ++i) {
    this->num_list[i] = this ->start + d*i;
24
26
28 }
```

Here is the caller graph for this function:

```
BaseSweeper::generate __num_list
```

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.

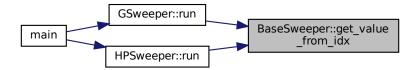
```
35
36 return start;
```

4.5.3.5 get_value_from_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()

this -> CUDA_use=true;
this -> gpu_num = gpu_num;
this -> gpu_limit = gpu_limit;

Here is the caller graph for this function:



4.5.3.7 set_MPI_info()

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()

58 this -> print_info = print_info;

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.

```
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.

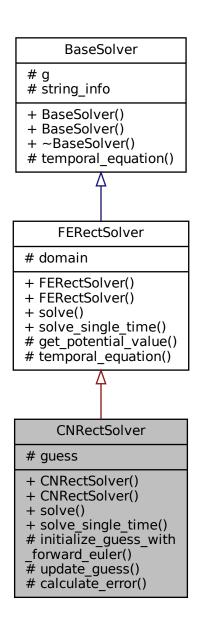
The documentation for this class was generated from the following files:

- /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

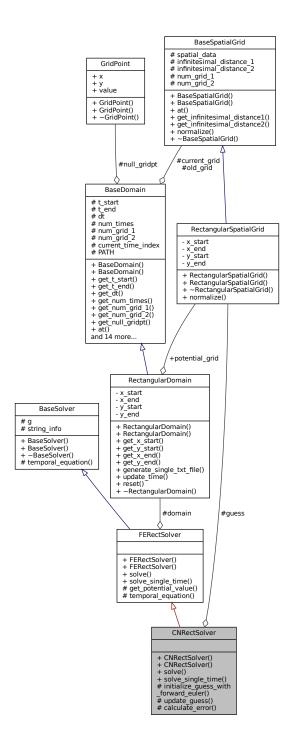
4.6 CNRectSolver Class Reference

#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]

```
{\tt CNRectSolver::CNRectSolver ( ) [default]}
```

4.6.2.2 CNRectSolver() [2/2]

```
\label{eq:cnrectSolver} \begin{split} \text{CNRectSolver::CNRectSolver} & ( \\ & \text{float } g, \\ & \text{RectangularDomain * } \textit{domain} \ ) \end{split}
```

Construct a new CNRectSolver::CNRectSolver object.

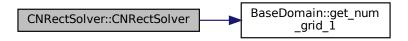
Parameters



Definition at line 20 of file cn_rect_solver.cpp.

```
: FERectSolver(g, domain) //
24 {
25
       // this->generate_potential_grid();
26
       this->guess = new RectangularSpatialGrid(
            this->domain->get_num_grid_1(),
28
           this->domain->get_num_grid_2(),
29
           this->domain->get_x_start(),
           this->domain->get_x_end(),
30
           this->domain->get_y_start(),
this->domain->get_y_end());
31
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()

Calculate L2 error between the ccurrent and previous guess.

Parameters



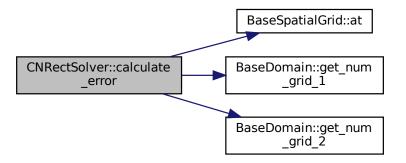
Returns

float

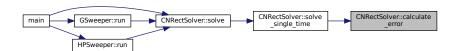
Definition at line 94 of file cn_rect_solver.cpp.

```
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)
```

Here is the call graph for this function:



Here is the caller graph for this function:



4.6.3.2 get_potential_value()

Get Potential value on each grid point.

Parameters

i	
j	

Returns

float

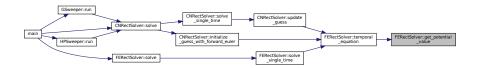
Definition at line 37 of file fe_rect_solver.cpp.

```
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()

```
\label{local_constraint} \mbox{void CNRectSolver::initialize\_guess\_with\_forward\_euler (} \\ \mbox{int $k$ ) [protected]}
```

initialize guess with forward euler method

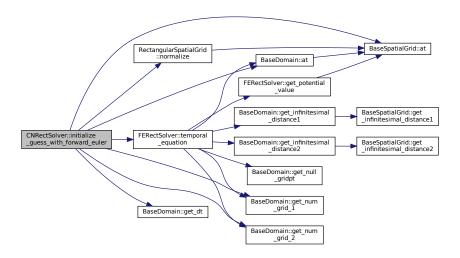
Parameters



Definition at line 41 of file cn_rect_solver.cpp.

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

Here is the call graph for this function:



Here is the caller graph for this function:



4.6.3.4 solve() [1/2]

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

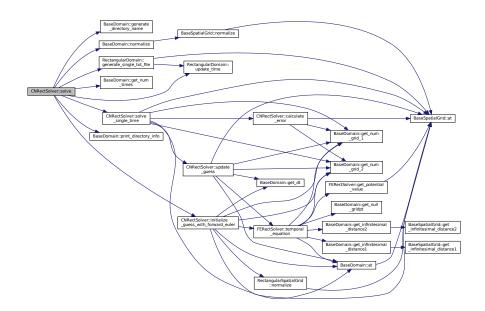
Parameters

tolerance	
max_iter	
dir_name	
print_info	
save_data	

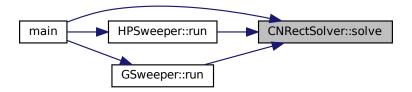
Definition at line 162 of file cn_rect_solver.cpp.

```
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
            this->domain->generate_single_txt_file(std::string("Solution_") + std::to_string(0));
169
170
        }else{
171
            this -> domain->update_time();
172
173
        for (int k = 0; k < time_length-1; ++k)
174
            //Update kth grid using k-1 th grid
// std::cout « "time step " « k « std::endl;
175
176
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.

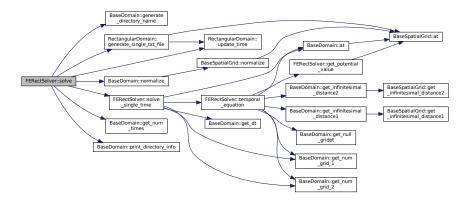
Parameters

	_
dir_name	
print_info	
save_data	

Definition at line 116 of file fe_rect_solver.cpp.

```
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
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){
                this->domain->generate_single_txt_file(std::string("Solution_") + std::to_string(k + 1));
132
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.

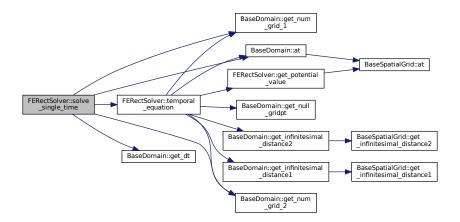
Parameters



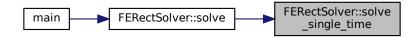
Definition at line 95 of file fe_rect_solver.cpp.

```
int Nx = this->domain->get_num_grid_1();
int Ny = this->domain->get_num_grid_2();
97
98
          float dt = this->domain->get_dt();
for (int i = 0; i < Nx; ++i)</pre>
99
100
101
102
                  for (int j = 0; j < Ny; ++j)
103
                        (\texttt{this->domain->at(i, j, k+1)->value}) \ = \ \texttt{this->domain->at(i, j, k)->value} \ + \ \texttt{dt} \ \star \\
104
          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

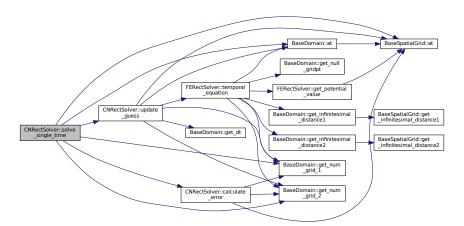
k	
tolerance	
max_iter	

Definition at line 114 of file cn_rect_solver.cpp.

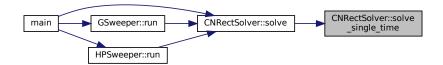
```
115 {
116     float error = 1.;
117     bool converged = false;
118     int converged_step = 0;
119     for (auto iter = 0; iter < max_iter; ++iter)</pre>
```

```
120
        {
121
             if (error < tolerance)</pre>
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
                 for (auto j = 0; j < this->domain->get_num_grid_2(); ++j)
130
131
                      this->domain->at(i, j, k)->value = this->guess->at(i, j)->value;
132
133
134
135
             //for each point, update predicted value
for (auto i = 0; i < this->domain->get_num_grid_1(); ++i)
136
137
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
             std::cout « "At time "«k «" Converged failed with error = " « error « std::endl;
149
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)

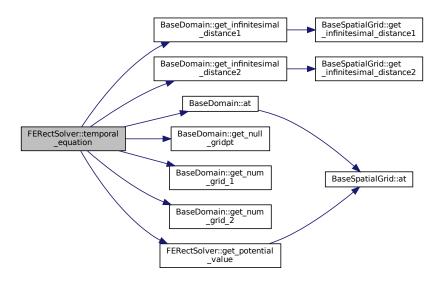
Returns

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

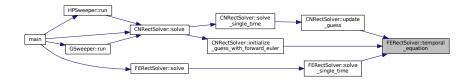
Definition at line 51 of file fe rect solver.cpp.

```
52 {
53
        //Use five stencil method
        auto point_data = this->domain->at(i, j, k);
54
5.5
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);
        if (i <= 0)
59
            point_data_l = this->domain->get_null_gridpt();
        auto point_data_d = this->domain->at(i, j - 1, k);
62
        if (j <= 0)
        point_data_d = this->domain->get_null_gridpt();
auto point_data_r = this->domain->at(i + 1, j, k);
if (i >= (this->domain->get_num_grid_1()) - 1)
63
64
65
            point_data_r = this->domain->get_null_gridpt();
        auto point_data_u = this->domain->at(i, j + 1, k);
if (j >= (this->domain->get_num_grid_2()) - 1)
68
69
             point_data_u = this->domain->get_null_gridpt();
70
71
        //potential at x, y
float V_ij = this->get_potential_value(i, j);
72
73
        //this->potential_func(point_data->x, point_data->y);
74
75
        //g * |psi(x,y)|^2
        float additional_term = (this->g) * (std::abs(point_data->value)) * (std::abs(point_data->value));
76
78
        //Set infinitesimal value
        float dx = this->domain->get_infinitesimal_distance1();
80
        float dy = this->domain->get_infinitesimal_distance2();
        //df denote time differential of dt (d(psi)/dt) // = (laplace - V-g|psi|^2) psi
81
82
        std::complex<float> df =
83
             +((point_data_r->value) + (point_data_l->value) - (point_data->value) * std::complex<float>{2}) /
        (\texttt{std::complex} < \texttt{float} > \{\texttt{dx} * \texttt{dx}\}) + ((\texttt{point\_data\_u} - \texttt{value}) + (\texttt{point\_data\_d} - \texttt{value}) - (\texttt{point\_data} - \texttt{value})
         * std::complex<float>{2}) / (std::complex<float>{dy * dy}) - (V_ij + additional_term) *
        (point_data->value);
8.5
        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()

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

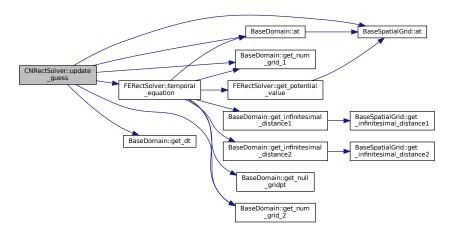
Parameters

i	
j	
k	

Definition at line 71 of file cn_rect_solver.cpp.

```
72 {
73
74
            for (auto i = 0; i < this->domain->get_num_grid_1(); ++i)
75
                   for (auto j = 0; j < this->domain->get_num_grid_2(); ++j)
76
                         this->guess->at(i, j)->value = (
    0.99f * this->guess->at(i, j)->value +
    0.01f * (
78
79
                                      this->domain->at(i, j, k - 1)->value +
std::complex<float>{0.5, 0.} * this->domain->get_dt() * (
    this->temporal_equation(i, j, k - 1) +
    this->temporal_equation(i, j, k)))); // this->temporal_equation_from_guess(i,
80
81
82
83
            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
- $\bullet \ \ / home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/solver/serial_solver/crank_nicolson/cn_rect_solver.cpp$

4.7 ConfigParser Class Reference

Configuration parser.

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

Collaboration diagram for ConfigParser:

ConfigParser

- + ConfigParser()
- + ~ConfigParser()
- + parse()
- + get_default()

Public Member Functions

- ConfigParser ()=default
- virtual \sim 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.
```

```
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";
         domain_parameters.n_x = 256;
domain_parameters.n_y = 256;
domain_parameters.n_time = 5;
506
507
508
509
         domain_parameters.time_start = 0.;
510
         domain_parameters.time_end = 0.01;
         domain_parameters.spatial_parameters["x_start"] = -10.;
domain_parameters.spatial_parameters["x_end"] = 10.;
domain_parameters.spatial_parameters["y_start"] = -10.;
512
513
         domain_parameters.spatial_parameters["y_end"] = 10.;
514
515
516
         init_parameters.init_cond_type = "singlegaussian";
517
         init_parameters.init_cond_parameters["sigma_x"] = 1.;
         init_parameters.init_cond_parameters["sigma_y"] = 1.;
init_parameters.init_cond_parameters["center_x"] = 0.;
518
519
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.;
         equation_parameters.potential_parameters["omega_y"] = 5.;
525
526
         solver_parameters.method = "cranknicolson";
527
528
         solver_parameters.run_parallel = true;
529
         solver_parameters.print_info = false;
530
         solver_parameters.save_data = false;
         solver_parameters.solver_parameters["converge_crit"] = 1e-11;
solver_parameters.int_parameters["max_iter"] = 1001;
531
532
         solver_parameters.int_parameters["cuda_device"] = 0;
533
534
535
         parameters.main_parameters = main_parameters;
536
         parameters.domain_parameters = domain_parameters;
537
         parameters.init_cond_parameters = init_parameters;
         parameters.equation_parameters = equation_parameters;
parameters.solver_parameters = solver_parameters;
538
539
540
         return parameters;
541 }
```

Here is the caller graph for this function:



4.7.3.2 parse()

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.
```

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

```
76
                // Do action for each branches
                else{
// Handle exception
77
78
79
                    if (mode == -1) {
                        std::cerr « "Unexpected Configuration File" « std::endl;
80
81
82
                    // Main branch
83
                    else if(mode == 0){
84
                        std::vector<std::string> dump;
8.5
                        std::string tmp;
                        std::stringstream string_stream(line);
if (line.rfind("type", 0) != std::string::npos)
86
87
88
89
                             while (std::getline(string_stream, tmp, '='))
90
91
                                 dump.push_back(tmp);
92
                             if (dump.size() != 2)
93
94
                                 std::cerr « "Unexpected Configuration File" « std::endl;
96
97
                            main_parameters.calculation_type = dump[1];
98
                        }
99
                        else{
                              while (std::getline(string_stream, tmp, '='))
100
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
                              else if (dump[0] == "sweep_count")
116
117
                                  main_parameters.int_parameters[dump[0]] = std::atoi(dump[1].c_str());
118
119
120
                              else if (dump[0] == "end_point")
121
                                  if (dump[1] == "true")
122
123
124
                                      main_parameters.int_parameters[dump[0]] = (int)true;
125
                                  else if (dump[1] == "false")
126
127
128
                                      main_parameters.int_parameters[dump[0]] = (int)false;
129
130
                                  else
131
132
                                      std::cerr « "Unexpected Configuration File" « std::endl;
133
134
                              else if (dump[0] == "mpi_use")
135
136
137
                                  if (dump[1] == "true")
138
139
                                      main_parameters.int_parameters[dump[0]] = (int)true;
140
                                  else if (dump[1] == "false")
141
142
                                      main_parameters.int_parameters[dump[0]] = (int)false;
143
144
145
                                  else
146
                                      std::cerr « "Unexpected Configuration File" « std::endl;
147
148
149
150
                              else if (dump[0] == "cuda_use")
151
                                  if (dump[1] == "true")
152
153
                                      main_parameters.int_parameters[dump[0]] = (int)true;
154
155
                                  else if (dump[1] == "false")
156
157
158
                                      main_parameters.int_parameters[dump[0]] = (int)false;
159
160
                                  else
```

```
161
162
                                      std::cerr « "Unexpected Configuration File" « std::endl;
163
164
                             else if (dump[0] == "gpu_count")
165
166
                                  main_parameters.int_parameters[dump[0]] = std::atoi(dump[1].c_str());
167
168
169
                             else if (dump[0] == "calculation_per_gpu")
170
                                 main_parameters.int_parameters[dump[0]] = std::atoi(dump[1].c_str());
171
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;
                         std::stringstream string_stream(line);
if (line.rfind("type", 0) != std::string::npos)
183
184
185
                              while (std::getline(string_stream, tmp, '='))
186
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(
                              while (std::getline(string_stream, tmp, '='))
196
197
198
                                  dump.push_back(tmp);
199
200
                              if (dump.size() != 2)
201
                                  std::cerr « "Unexpected Configuration File" « std::endl;
202
203
204
                              if (domain_parameters.domain_type != ""){
205
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
                                  if (dump[0] == "n_x"){
215
                                      domain_parameters.n_x = std::atoi(dump[1].c_str());
216
218
                                  else if(dump[0] == "n_y"){
219
                                      domain_parameters.n_y = std::atoi(dump[1].c_str());
220
                                  else if(dump[0] == "n_time"){
221
                                      domain_parameters.n_time = std::atoi(dump[1].c_str());
222
223
                                  else if(dump[0] == "time_start"){
224
225
                                      domain_parameters.time_start = (float)std::atof(dump[1].c_str());
226
                                  else if(dump[0] == "time_end"){
227
                                      domain_parameters.time_end = (float)std::atof(dump[1].c_str());
228
229
                                  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
                     // initial condition branches
239
240
                     else if(mode == 2){
                         std::vector<std::string> dump;
241
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)
2.51
252
                                 std::cerr « "Unexpected Configuration File" « std::endl;
253
254
                              init_parameters.init_cond_type = dump[1];
255
256
                         else
257
                             while (std::getline(string_stream, tmp, '='))
258
259
260
                                 dump.push_back(tmp);
261
262
                              if (dump.size() != 2)
263
                                 std::cerr « "Unexpected Configuration File" « std::endl;
264
265
266
267
                              if (init_parameters.init_cond_type != "")
268
2.69
                                 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
                     // eqution branch
278
                     else if (mode == 3) {
279
                         std::vector<std::string> dump;
280
                         std::string tmp;
                         std::stringstream string_stream(line);
281
                         if (line.rfind("type", 0) != std::string::npos)
282
283
284
                              while (std::getline(string_stream, tmp, '='))
285
286
                                 dump.push_back(tmp);
2.87
288
                              if (dump.size() != 2)
289
290
                                 std::cerr « "Unexpected Configuration File" « std::endl;
291
292
                             equation_parameters.potential_type = dump[1];
293
                         else if (line.rfind("g", 0) != std::string::npos)
294
295
296
                              while (std::getline(string_stream, tmp, '='))
297
298
                                 dump.push_back(tmp);
299
300
                              if (dump.size() != 2)
301
                                 std::cerr « "Unexpected Configuration File" « std::endl;
302
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
                              if (dump.size() != 2)
312
313
314
                                 std::cerr « "Unexpected Configuration File" « std::endl;
315
316
317
                              if (equation_parameters.potential_type != "")
318
                                 equation_parameters.potential_parameters[dump[0]] =
319
       std::atof(dump[1].c_str());
320
321
322
                                 std::cerr « "Unexpected Configuration File" « std::endl;
323
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
                         if (line.rfind("method", 0) != std::string::npos)
334
335
336
                             while (std::getline(string_stream, tmp, '='))
337
338
                                 dump.push_back(tmp);
339
340
                             if (dump.size() != 2)
341
                                 std::cerr « "Unexpected Configuration File" « std::endl;
342
343
344
                             solver_parameters.method = dump[1];
345
346
347
                         // Get Parallel
                         else if (line.rfind("parallel", 0) != std::string::npos)
348
349
350
                             while (std::getline(string_stream, tmp, '='))
351
352
                                 dump.push_back(tmp);
353
                             if (dump.size() != 2)
354
355
356
                                 std::cerr « "Unexpected Configuration File" « std::endl;
357
358
359
                             if (dump[1].rfind("true", 0) != std::string::npos)
360
                                 solver_parameters.run_parallel = true;
361
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
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
                             if (dump.size() != 2)
381
382
383
                                 std::cerr « "Unexpected Configuration File" « std::endl;
384
385
                             if (dump[1].rfind("true", 0) != std::string::npos)
386
                                 solver_parameters.print_info = true;
387
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
                             if (dump.size() != 2)
406
407
408
                                 std::cerr « "Unexpected Configuration File" « std::endl;
409
                             if (dump[1].rfind("true", 0) != std::string::npos)
410
411
                                 solver parameters.save data = true;
412
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
                        else if (line.rfind("cuda_device", 0) != std::string::npos)
425
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
                             solver_parameters.int_parameters[dump[0]] = std::atoi(dump[1].c_str());
435
436
437
438
                        // Get max iter
439
                        else if (line.rfind("max_iter", 0) != std::string::npos)
440
                             while (std::getline(string_stream, tmp, '='))
441
442
443
                                 dump.push_back(tmp);
444
445
                             if (dump.size() != 2)
446
                                 std::cerr « "Unexpected Configuration File" « std::endl;
447
448
449
                             solver_parameters.int_parameters[dump[0]] = std::atoi(dump[1].c_str());
450
                        }
451
452
                        else
453
                             while (std::getline(string_stream, tmp, '='))
454
455
456
                                 dump.push_back(tmp);
457
458
                             if (dump.size() != 2)
459
                                 std::cerr « "Unexpected Configuration File" « std::endl;
460
461
                             if ( (solver_parameters.method != "") && filled_parallel)
462
463
464
                                 solver_parameters.solver_parameters[dump[0]] = std::atof(dump[1].c_str());
465
466
                             else
467
                             {
                                 std::cerr « "Unexpected Configuration File" « std::endl;
468
469
470
471
472
473
                     else{
                        std::cerr « "Unexpected Configuration File" « std::endl;
474
475
476
                }
477
478
        // setup parameters
479
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:

DomainParameters + domain_type + n_x + n_y + n_time + spatial_parameters + time_start + time_end

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

```
\verb|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:

+ g + potential_type + potential_parameters

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:

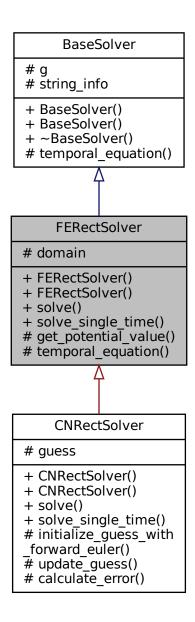
 $\bullet \ \ / home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/parameters.h$

4.10 FERectSolver Class Reference

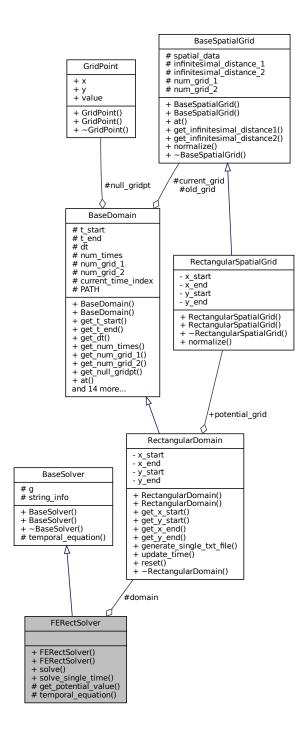
Forward Euler Serial Solver.

```
#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 ( \label{float} float \ g\_, \\ \\ RectangularDomain * domain\_ )
```

Construct a new FERectSolver::FERectSolver object.

Parameters

<i>g_</i>	
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



Returns

float

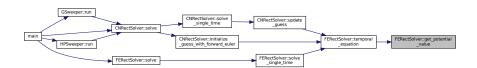
Definition at line 37 of file fe_rect_solver.cpp.

```
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.

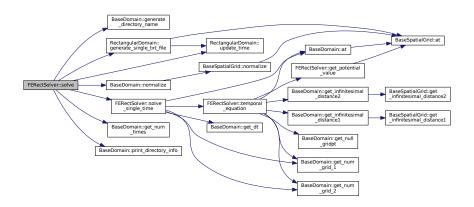
Parameters

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
             this->domain->generate_single_txt_file(std::string("Solution_") + std::to_string(0));
122
123
        }else{
124
             this -> domain->update_time();
125
126
127
        for (int k = 0; k < time_length - 1; ++k)
128
             this->solve_single_time(k);
this->domain->normalize(k + 1);
129
130
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 )
```

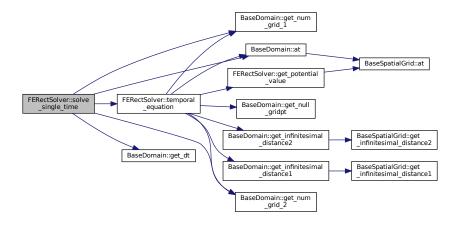
Update k+1 th wave function value with k th values.

Parameters



Definition at line 95 of file fe_rect_solver.cpp.

Here is the call graph for this function:



Here is the caller graph for this function:



4.10.3.4 temporal_equation()

```
\begin{tabular}{ll} {\tt std::complex}< & {\tt float} > {\tt FERectSolver::temporal\_equation} & ( & {\tt int} i, & \\ & & {\tt int} j, & \\ & & {\tt int} k \end{tabular} \label{eq:complex}
```

Time differential of phi.

Parameters

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

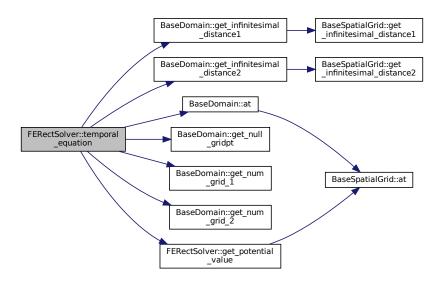
Returns

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

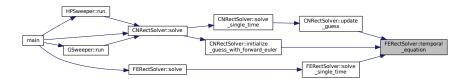
Definition at line 51 of file fe_rect_solver.cpp.

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

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:

GridPoint + x + y + value + GridPoint() + GridPoint() + ~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]

Definition at line 13 of file base_domain.cpp.

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

4.11.2.3 ∼GridPoint()

```
GridPoint:: \sim 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.

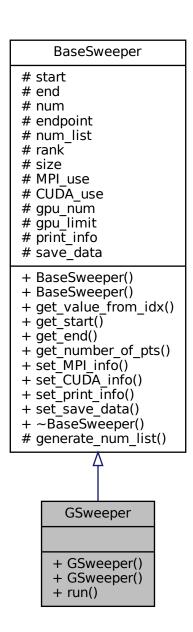
The documentation for this class was generated from the following files:

- /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

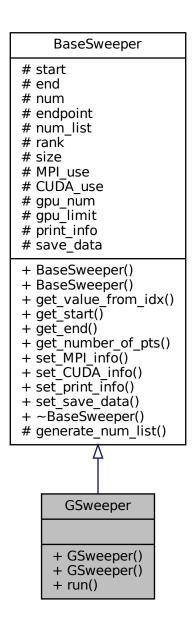
4.12 GSweeper Class Reference

#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]

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.

```
this->num_list = std::vector<float>(this->num);
float d = 0.;
if(this->endpoint){
    d = (this -> end - this-> start ) / float(this-> num -1 );
}else{
    d = (this -> end - this-> start ) / float(this-> num);
}

for (int i=0; i<this -> num; ++i){
    this->num_list[i] = this -> start + d*i;
}

this->num_list[i] = this -> start + d*i;
}
```

Here is the caller graph for this function:

```
BaseSweeper::BaseSweeper _____ BaseSweeper::generate __num_list
```

4.12.3.2 get_end()

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

Definition at line 38 of file base sweeper.cpp.

4.12.3.3 get_number_of_pts()

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

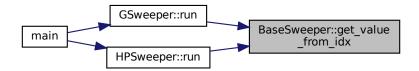
```
Definition at line 41 of file base_sweeper.cpp.
```

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

4.12.3.4 get_start()

4.12.3.5 get_value_from_idx()

Here is the caller graph for this function:



4.12.3.6 run()

void GSweeper::run (

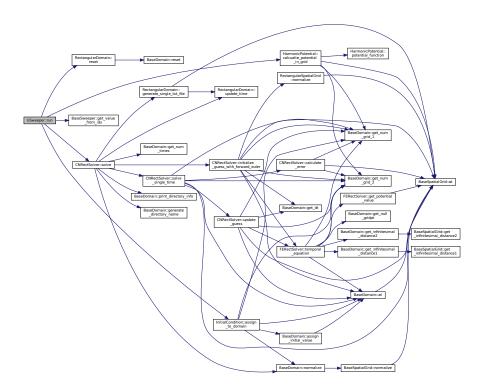
```
InitialCondition * initial_condition,
               HarmonicPotential * potential )
Definition at line 12 of file g_sweeper.cpp.
12
13
14
       if (!(this -> MPI_use) && !(this -> CUDA_use)){
           if(print_info){
    cout« "Running serially started"«endl;
17
18
            float g=0;
19
            for(int i=0; i<this -> num ; ++i){
20
                //Set conditions
                initial_condition->assign_to_domain(domain);
23
                potential->calcualte_potential_in_grid(domain);
24
                g = this -> get_value_from_idx(i);
//Apply on solver
25
26
                CNRectSolver* solver = new CNRectSolver(g, domain);
```

//solve using solver. It automatically save data

RectangularDomain * domain,

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

54

Here is the caller graph for this function:



4.12.3.8 set_MPI_info()

Definition at line 45 of file base_sweeper.cpp.

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.

```
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.

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.

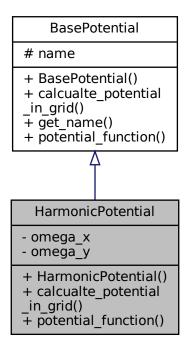
The documentation for this class was generated from the following files:

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

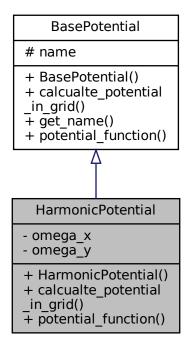
4.13 HarmonicPotential Class Reference

#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()

```
\label{eq: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



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 }
```

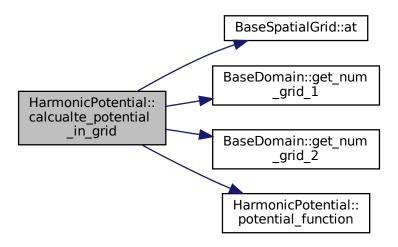
4.13.3 Member Function Documentation

4.13.3.1 calcualte potential in grid()

Definition at line 29 of file harmonic_potential.cpp.

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

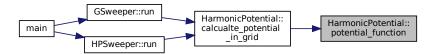
```
41 {
42 return this->name;
```

4.13.3.3 potential_function()

Definition at line 25 of file harmonic_potential.cpp.

```
20     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.

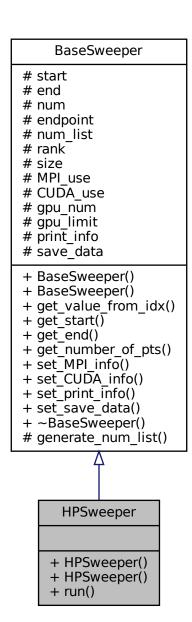
The documentation for this class was generated from the following files:

- /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

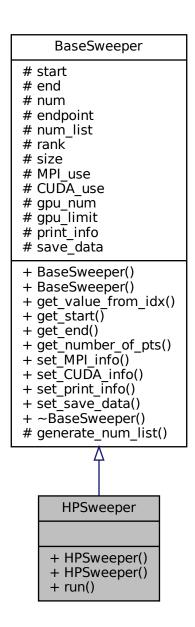
4.14 HPSweeper Class Reference

#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]

Definition at line 7 of file harmonic_p_sweeper.cpp.

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

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.

```
this->num_list = std::vector<float>(this->num);
float d = 0.;
if(this->endpoint){
    d = (this -> end - this-> start ) / float(this-> num -1 );
}else{
    d = (this -> end - this-> start ) / float(this-> num);
}

for (int i=0; i<this -> num; ++i){
    this->num_list[i] = this -> start + d*i;
}

this->num_list[i] = this -> start + d*i;
}
```

Here is the caller graph for this function:

```
BaseSweeper::BaseSweeper _____ BaseSweeper::generate __num_list
```

4.14.3.2 get_end()

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

Definition at line 38 of file base sweeper.cpp.

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.

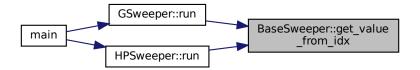
```
35
36    return start;
37 }
```

4.14.3.5 get_value_from_idx()

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:



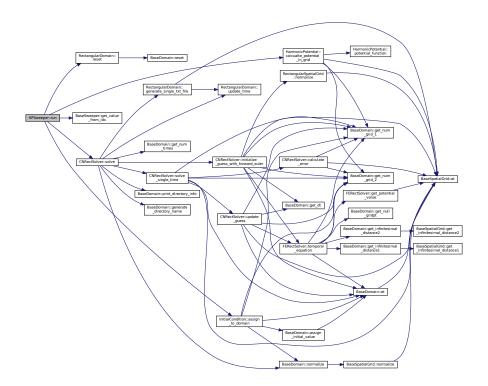
4.14.3.6 run()

Definition at line 12 of file harmonic_p_sweeper.cpp.

```
13
14
        if (!(this -> MPI_use) && !(this -> CUDA_use)){
15
             if(print_info){
17
                 cout« "Running serially started"«endl;
18
19
             for(int i=0; i<this -> num ; ++i){
20
                 //Set conditions
                 initial_condition->assign_to_domain(domain);
                 HarmonicPotential * potential = new HarmonicPotential(1, get_value_from_idx(i));
potential->calcualte_potential_in_grid(domain);
24
                 g = this -> get_value_from_idx(i);
//Apply on solver
2.5
26
                 CNRectSolver* solver = new CNRectSolver(g, domain);
                 //solve using solver. It automatically save data
```

```
solver->solve(le-11, 101, to_string(i) , this-> print_info, this -> save_data);
                  //reset domain to use in next iteration
30
31
                 domain->reset();
32
                 delete solver;
33
                 delete potential;
34
            }
35
        else if ((this->MPI_use) && !(this->CUDA_use)){
36
37
            //If number of tasks exceed number of processors, abort.
38
             if(print_info){
                 cout« "Running with only MPI started"«endl;
39
40
             if (num > size) {
41
                 MPI_Abort ( MPI_COMM_WORLD, EXIT_FAILURE);
42
43
44
             float g = 0;
            if (rank < num) {</pre>
45
                 initial condition->assign to domain(domain);
46
                 HarmonicPotential * potential = new HarmonicPotential(1, get_value_from_idx(rank));
                 potential -> calcualte_potential_in_grid(domain);
                 CNRectSolver* solver = new CNRectSolver(g, domain); solver->solve(le-11, 101, "MPI_"+to_string(rank), this -> print_info, this->save_data);
49
50
51
                 delete solver;
52
                 delete potential;
             }else{
53
                 // No job for extra processors
55
56
        }else if (!(this->MPI_use) && (this->CUDA_use)){
57
58
59
             if(print_info){
                 cout« "Running with CUDA serially started" «endl;
60
62
             for(int i=0; i<this -> num ; ++i){
63
                 //Set conditions
64
                 initial_condition->assign_to_domain(domain);
                 HarmonicPotential * potential = new HarmonicPotential(1, get_value_from_idx(i)); potential->calcualte_potential_in_grid(domain);
65
66
                  //Apply on solver
68
                 CNRectPSolver* solver = new CNRectPSolver(g, domain, 0);//solve using solver. It automatically
        save data
                 solver->solve(le-11, 101, "CUDA_"+to_string(i) , this-> print_info, this -> save_data);
69
70
                 //reset domain to use in next iteration
                 domain->reset();
72
                 delete solver;
73
                 delete potential;
74
            }
7.5
76
77
        else{
78
             if (print_info) {
79
                 cout« "Running with CUDA & MPI started" «endl;
80
81
             float q=0;
82
83
             if (num > size) {
                 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);
             for(int i=0; i<repeat; ++i){</pre>
88
                 if (i*repeat < max_pallel_tasks && rank < (i+1)*max_pallel_tasks && rank < num ){
  int casted_GPU_num = (rank % max_pallel_tasks) % gpu_limit;</pre>
89
90
                      initial_condition->assign_to_domain(domain);
92
                      auto potential = new HarmonicPotential(1, get_value_from_idx(rank));
93
                      potential->calcualte_potential_in_grid(domain);
                      //g = this -> get_value_from_idx(rank);
CNRectPSolver* solver =new CNRectPSolver(g, domain, casted_GPU_num);
solver->solve(le-11, 101, "MPI&CUDA_"+to_string(rank), this -> print_info,
94
95
96
        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
        this -> CUDA_use=true;
this -> gpu_num = gpu_num;
this -> gpu_limit = gpu_limit;
52
53
```

54

Here is the caller graph for this function:



4.14.3.8 set_MPI_info()

Definition at line 45 of file base_sweeper.cpp.

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:

InitialCondition

- initial_condition_function
- + InitialCondition()
- + InitialCondition()
- + assign_to_domain()

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]

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()

Assign initial condition to the domain class instance.

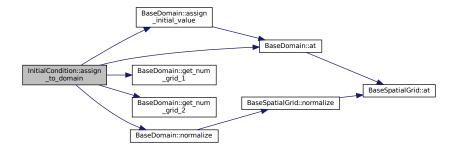
Parameters

domain

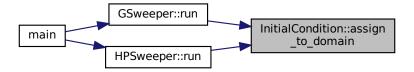
Definition at line 28 of file initial_condition.cpp.

```
30
        for (auto i = 0; i < domain->get_num_grid_1(); ++i)
31
32
33
             for (auto j = 0; j < domain->get_num_grid_2(); ++j)
34
                 auto point_data = domain->at(i, j, 0);
domain->assign_initial_value(i, j, this->initial_condition_function(point_data->x,
35
36
        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:

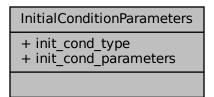
- $\bullet \ \ / home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/initial_condition/initial_condition.h$
- $\bullet \ \ / home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/initial_condition/initial_condition.cpp$

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:

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

4.17 MainParameters Class Reference

Main branch parameters containing information about overall calculation.

#include <parameters.h>

Collaboration diagram for MainParameters:

MainParameters

- + calculation_type
- + float_parameters
- + int parameters

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:

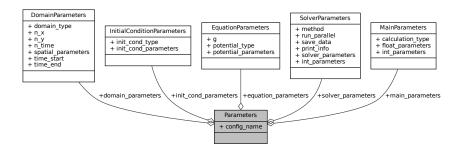
 $\bullet \ \ / home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/parameters.h$

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:

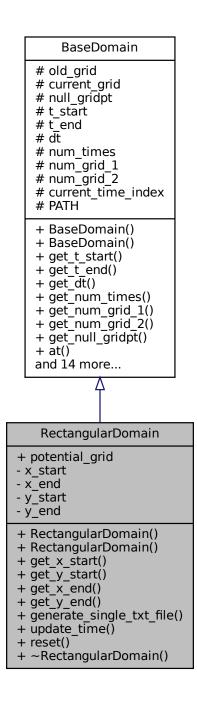
• /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/configuration/parameters.h

4.19 RectangularDomain Class Reference

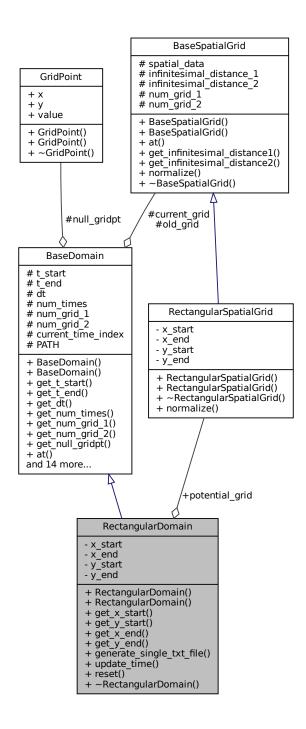
Rectangular domain containing multiple timesteps.

```
#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 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.
```

```
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::\simRectangularDomain ( )
```

```
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.
```

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.

Here is the call graph for this function:



4.19.3.3 at()

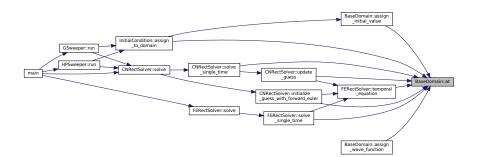
```
GridPoint * BaseDomain::at (
              int index_1,
              int index_2,
              int time_index ) [inherited]
Definition at line 153 of file base domain.cpp.
```

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

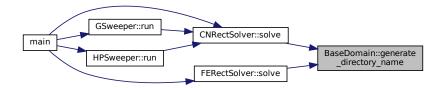
Returns

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;
        oss « std::put_time(&tm, "%Y-%m-%d-%H-%M-%S");
209
210
        auto str = oss.str();
        std::string directory_name = "../results/" + str + "_" + info;
211
212
        bool created = fs::create_directory(directory_name.c_str());
213
        if (print_info && created)
214
            std::cout « "Created directory " « directory_name « std::endl;
215
216
        // else if(print_info )
217
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:

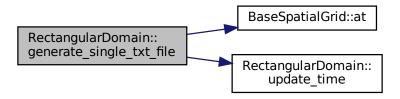


4.19.3.5 generate_single_txt_file()

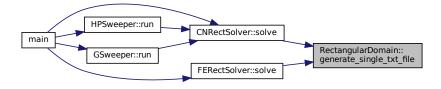
Definition at line 152 of file rect_domain.cpp.

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

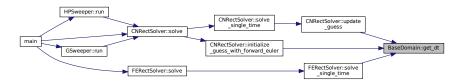
4.19.3.7 get_dt()

```
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]
```

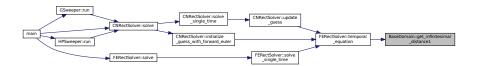
Definition at line 143 of file base_domain.cpp.

```
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]
```

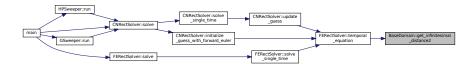
Definition at line 147 of file base_domain.cpp.

```
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:



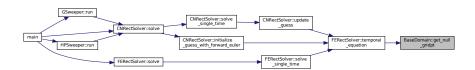
4.19.3.10 get_null_gridpt()

```
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:



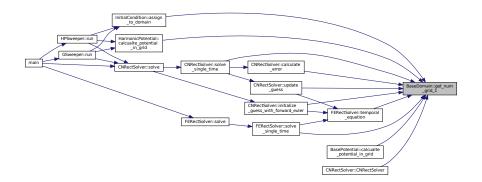
4.19.3.11 get_num_grid_1()

```
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:

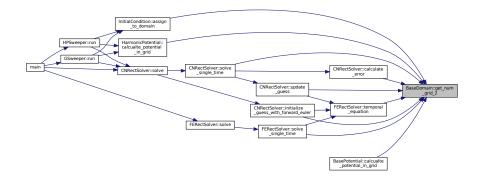


4.19.3.12 get_num_grid_2()

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

Definition at line 138 of file base_domain.cpp.

Here is the caller graph for this function:



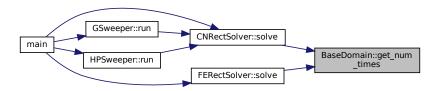
4.19.3.13 get_num_times()

```
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.

4.19.3.16 get_t_start()

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

Definition at line 116 of file base_domain.cpp.

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.

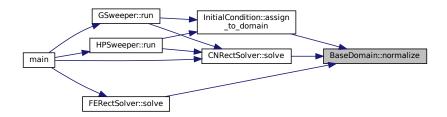
```
125 {
126         return this->y_start;
127 }
```

4.19.3.21 normalize()

Here is the call graph for this function:



Here is the caller graph for this function:



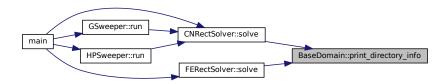
4.19.3.22 print_directory_info()

```
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.

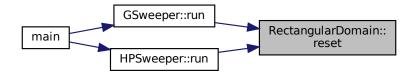
Definition at line 180 of file rect_domain.cpp.

```
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()

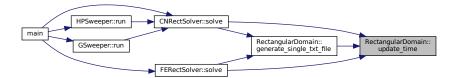
4.19.3.25 update_time()

```
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;
             delete (this->old_grid);
this->old_grid = this->current_grid;
146
147
             this->current_grid = new RectangularSpatialGrid(num_grid_1, num_grid_2, x_start, x_end, y_start,
148
       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

```
{\tt RectangularSpatialGrid*} \ {\tt 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

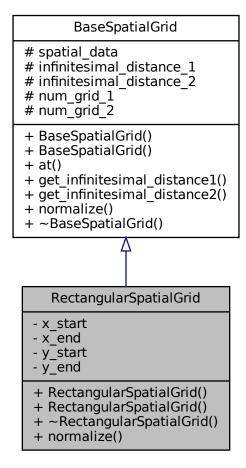
Rectangular Spatial Grid class for single time step.

#include <rect_domain.h>

Inheritance diagram for RectangularSpatialGrid:

BaseSpatialGrid # spatial data # infinitesimal_distance_1 # infinitesimal_distance_2 # num_grid_1 # num_grid_2 + BaseSpatialGrid() + BaseSpatialGrid() + get_infinitesimal_distance1() + get_infinitesimal_distance2() + normalize() + ~BaseSpatialGrid() RectangularSpatialGrid - x start x_end y_start - y_end + RectangularSpatialGrid() + RectangularSpatialGrid() + ~RectangularSpatialGrid() + normalize()

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 {
        this->x_start = x_start;
35
        this->x_end = x_end;
        this->y_start = y_start;
this->y_end = y_end;
//infinitesimal_distance 1,2 = dx, dy
36
37
38
        this->infinitesimal_distance_1 = (x_end - x_start) / (num_grid_1 - 1);
this->infinitesimal_distance_2 = (y_end - y_start) / (num_grid_2 - 1);
39
40
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)</pre>
43
             for (auto j = 0; j < num_grid_2; ++j)</pre>
44
45
                  this->spatial_data[i][j] = GridPoint(this->x_start + infinitesimal_distance_1 * i,
                                                                 this->y_start + infinitesimal_distance_2 * j,
47
                                                                 //{real value, imaginary value}
48
                                                                 std::complex<float>{0, 0});
49
50
             }
51
        }
```

4.20.2.3 ∼RectangularSpatialGrid()

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

```
Definition at line 76 of file rect_domain.cpp.
```

77 78 };

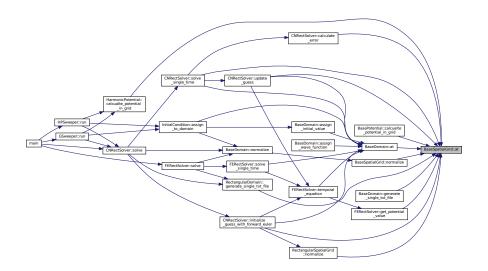
4.20.3 Member Function Documentation

4.20.3.1 at()

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.

```
/1 {
    return this->infinitesimal_distance_2;
73 }
```

Here is the caller graph for this function:

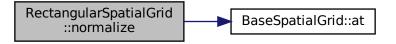


4.20.3.4 normalize()

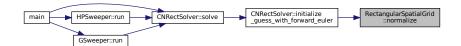
```
void RectangularSpatialGrid::normalize ( )
```

Definition at line 53 of file rect_domain.cpp.

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

 $\verb|float RectangularSpatialGrid::x_end [private]|\\$

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:

SolverParameters

- + method
- + run parallel
- + save data
- + print_info
- + solver_parameters
- + int parameters

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()

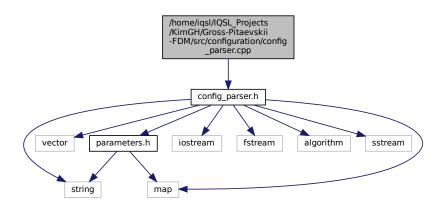
14 include_directories(\${MPI_INCLUDE_PATH})

5.1.1.2 target_link_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

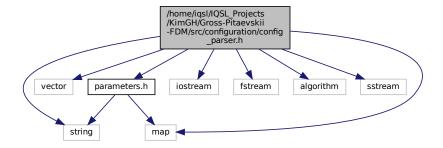
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5.3 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/configuration/config_parser.h File Reference

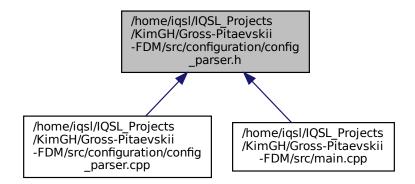
Configuration Parser Class header.

```
#include <string>
#include <vector>
#include <map>
#include <iostream>
#include <fstream>
#include <algorithm>
#include <sstream>
#include <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

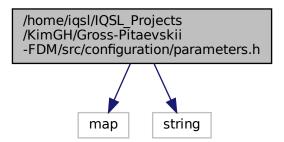
Copyright

Copyright (c) 2022

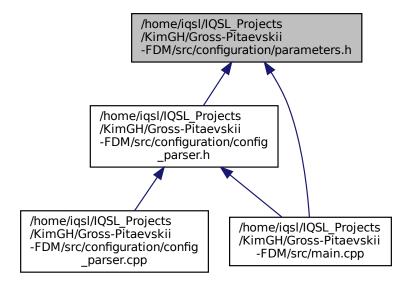
5.4 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/configuration/parameters.h File Reference

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

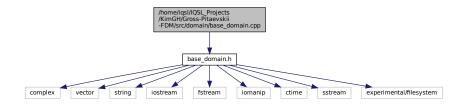
Copyright

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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

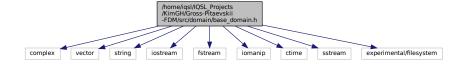
Copyright

Copyright (c) 2022

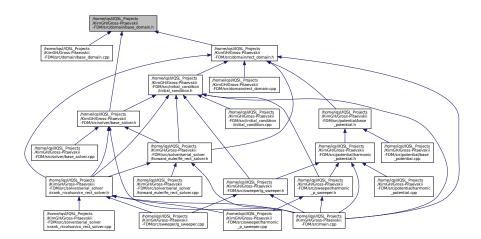
/home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/domain/base_domain.h File Reference

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

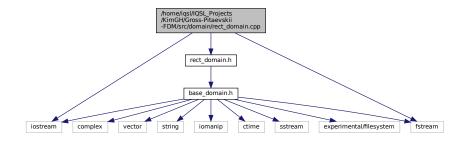
Copyright (c) 2022

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

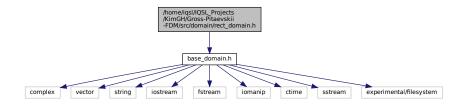
Copyright

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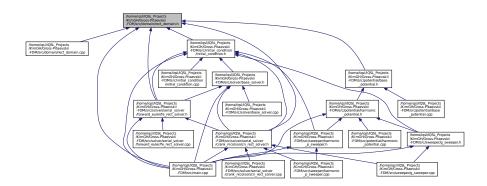
5.8 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD⊸ M/src/domain/rect_domain.h File Reference

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

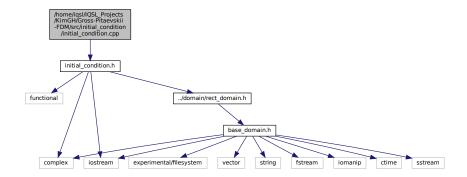
Copyright

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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

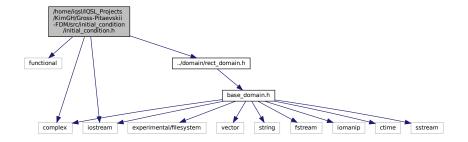
Copyright

Copyright (c) 2022

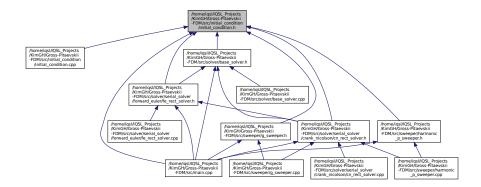
5.10 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FDM/src/initial __condition/initial_condition.h File Reference

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

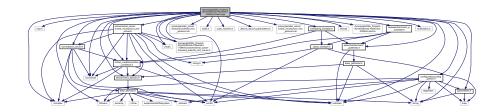
Copyright

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/home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/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.

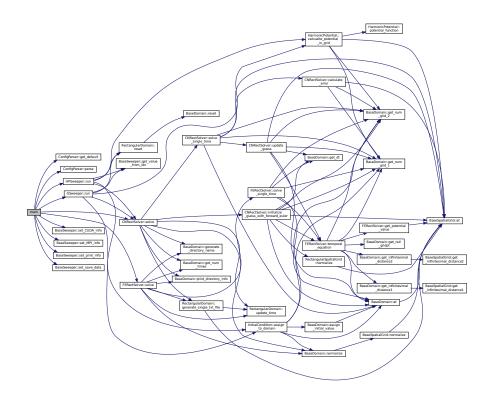
```
20
       //Initialize MPI
21
       MPI_Init(&argc, &argv);
22
       int rank, size;
       MPI_Comm comm = MPI_COMM_WORLD;
24
       MPI_Comm_rank(comm, &rank);
25
      MPI_Comm_size(comm, &size);
26
      Parameters parameters;
28
       // If argc == 1: no input configuration => use default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

```
31
            parameters = ConfigParser::get_default();
32
        // argc != 1 and argc != 2 => exception
33
        else if (argc != 2) {
34
            std::cerr « "Input config file required. " « std::endl;
35
36
37
        // else: use given configuration
38
        else{
            std::string config_filename = std::string(argv[1]);
std::size_t dir_pos = config_filename.find_last_of("/");
std::string dir = config_filename.substr(0, dir_pos);
39
40
41
             std::string config_name_extension = config_filename.substr(dir_pos + 1,
42
        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
             // Single calculation
51
            if (parameters.main_parameters.calculation_type == "single")
53
                  // 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 initial condition
                 std::function<std::complex<float>(float, float)> initial_cond_function;
if (parameters.init_cond_parameters.init_cond_type == "singlegaussian")
65
66
68
                      auto sigma_x = parameters.init_cond_parameters.init_cond_parameters["sigma_x"];
                      auto sigma_y = parameters.init_cond_parameters.init_cond_parameters["sigma_y"];
69
                      auto center_x = parameters.init_cond_parameters.init_cond_parameters["center_x"];
auto center_y = parameters.init_cond_parameters.init_cond_parameters["center_y"];
70
71
72
                      initial_cond_function = [center_x, center_y, sigma_x, sigma_y](float x, float y)
73
                           return std::complex<float>{
                               float(1.) * expf(-((x - center_x) * (x - center_x) / (sigma_x * sigma_x) + (y - center_x))
75
        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
                 {
                      std::cerr « "Unexpected initial condition" « std::endl;
84
86
                 // Prepare potential
87
88
                 if (parameters.equation_parameters.potential_type == "harmonic")
89
                      auto omega_x = parameters.equation_parameters.potential_parameters["omega_x"];
auto omega_y = parameters.equation_parameters.potential_parameters["omega_y"];
auto *potential = new HarmonicPotential(omega_x, omega_y);
90
91
                      potential->calcualte_potential_in_grid(domain);
93
94
9.5
                 // Library user could add case in here if they want to use non-harmonic potential
96
                 else
                 {
                      std::cerr « "Unexpected initial condition" « std::endl;
aa
100
101
                  float g = parameters.equation_parameters.g;
102
                  bool save_data = parameters.solver_parameters.save_data;
103
104
                  bool print_info = parameters.solver_parameters.print_info;
105
                  // Solve equation in given method from configuration
if (parameters.solver_parameters.method == "cranknicolson")
106
107
108
109
                       if(parameters.solver_parameters.run_parallel){
                            float converge_crit =
110
        parameters.solver_parameters.solver_parameters["converge_crit"];
```

```
int max_iter = parameters.solver_parameters.int_parameters["max_iter"];
111
                          int cuda_device = parameters.solver_parameters.int_parameters["cuda_device"];
CNRectPSolver solver = CNRectPSolver(g, domain, cuda_device);
112
113
114
                          solver.solve(converge_crit, max_iter, std::to_string(rank), print_info, save_data);
115
117
                          float converge_crit =
       parameters.solver_parameters.solver_parameters["converge_crit"];
118
                          int max_iter = parameters.solver_parameters.int_parameters["max_iter"];
CNRectSolver solver = CNRectSolver(g, domain);
119
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
                 else if (parameters.solver_parameters.method == "forwardeuler") {
124
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
                      {
                          FERectSolver solver = FERectSolver(g, domain);
133
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"],
                                                 parameters.main_parameters.float_parameters["sweep_end"], parameters.main_parameters.int_parameters["sweep_count"],
142
143
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
                 \verb|std::function<std::complex<float>(float, float)> initial\_cond\_function||;
                 if (parameters.init_cond_parameters.init_cond_type == "singlegaussian")
158
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"];
                      auto center_y = parameters.init_cond_parameters.init_cond_parameters["center_y"];
164
165
                      initial_cond_function = [center_x, center_y, sigma_x, sigma_y](float x, float y)
166
                          return std::complex<float>{
167
                              float(1.) * expf(-((x - center_x) * (x - center_x) / (sigma_x * sigma_x) + (y - center_x))
168
       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);
                          potential->calcualte_potential_in_grid(domain);
179
180
181
                          bool save_data = parameters.solver_parameters.save_data;
                          bool print_info = parameters.solver_parameters.print_info;
bool cuda_use = (bool)parameters.main_parameters.int_parameters["cuda_use"];
182
183
                          bool mpi_use = (bool)parameters.main_parameters.int_parameters["mpi_use"];
184
185
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
                                      else
203
204
205
                                              std::cerr « "Unexpected initial condition" « std::endl;
206
207
208
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"],
                                                                                            parameters.main_parameters.float_parameters["sweep_end"],
217
                                                                                            parameters.main_parameters.int_parameters["sweep_count"],
218
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
                              \verb|std::function| < \verb|std::complex| < float| < float, float| > initial\_cond\_function; \\
2.31
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"];
                                      auto center_x = parameters.init_cond_parameters.init_cond_parameters["center_x"];
auto center_y = parameters.init_cond_parameters.init_cond_parameters["center_y"];
237
238
239
                                       initial_cond_function = [center_x, center_y, sigma_x, sigma_y](float x, float y)
240
241
                                              return std::complex<float>{
2.42
                                                    {\tt float(1.)} \; \star \; {\tt expf(-((x - center\_x) \; \star \; (x - center\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (y - center\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (y - center\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (y - center\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (y - center\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (y - center\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (y - center\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (y - center\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (y - center\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (y - center\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (sigma\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (sigma\_x) \; / \; (sigma\_x \; \star \; sigma\_x) \; + \; (sigma\_x) \; / \;
             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
                                              // setup save / MPI use / cuda use / print option
249
                                              float g = parameters.equation_parameters.g;
250
                                              bool save_data = parameters.solver_parameters.save_data;
bool print_info = parameters.solver_parameters.print_info;
251
252
                                              bool cuda_use = (bool)parameters.main_parameters.int_parameters["cuda_use"];
bool mpi_use = (bool)parameters.main_parameters.int_parameters["mpi_use"];
253
254
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
                                                     hpSweeper.set_MPI_info(rank, size);
262
263
                                              hpSweeper.set_print_info(print_info);
264
265
                                              hpSweeper.set_save_data(save_data);
266
267
                                              hpSweeper.run(domain, initial_condition, g);
268
269
                                      else
270
```

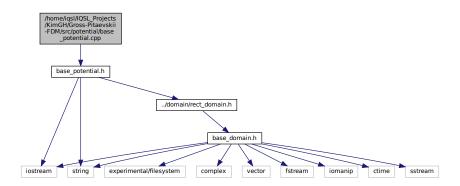
Here is the call graph for this function:



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

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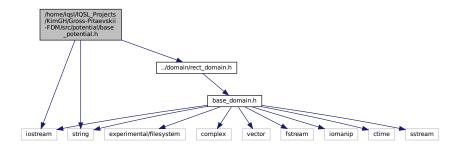
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5.13 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/potential/base_potential.h File Reference

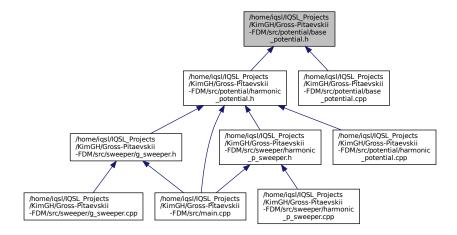
Header for the base potential class. Heritate this class for create custom potential shape.

```
#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

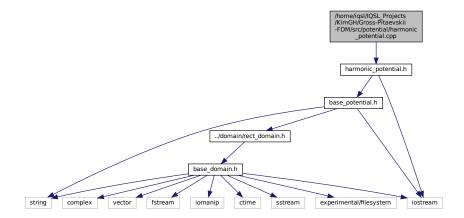
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Copyright (c) 2022

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

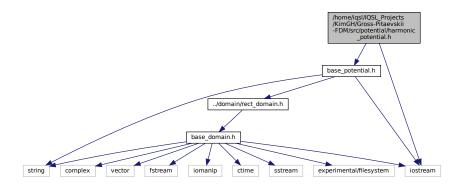
Copyright (c) 2022

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

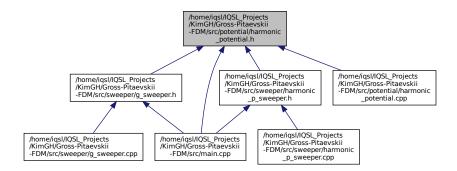
Header file for harmoni potential (V = 0.5 * (omega $x^2 * x^2 + omega y^2 * y^2$)

#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

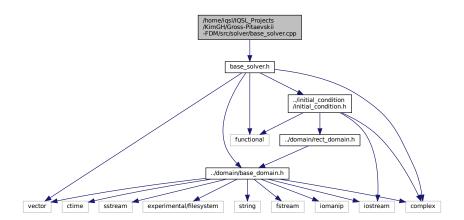
Copyright

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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

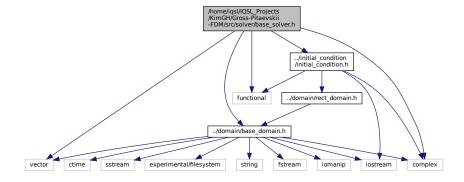
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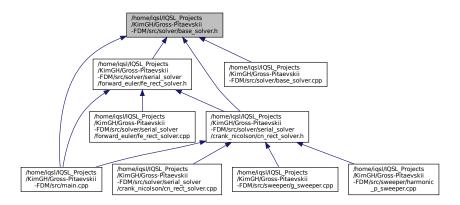
5.17 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/solver/base_solver.h File Reference

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

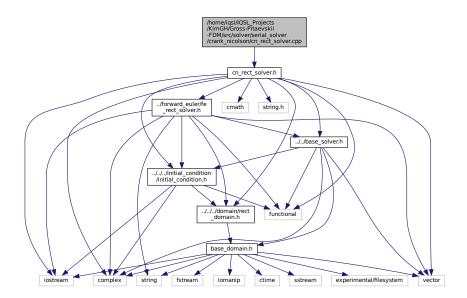
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5.18 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/solver/serial_solver/crank_nicolson/cn_rect_solver.cpp File Reference

Implementation file for serial crank nicolson solver.

#include "cn_rect_solver.h"
Include dependency graph for cn_rect_solver.cpp:



Reference 175

5.18.1 Detailed Description

Implementation file for serial crank nicolson solver.

Author

Minyoung Kim, Gyeonghun Kim

Version

0.1

Date

2022-06-05

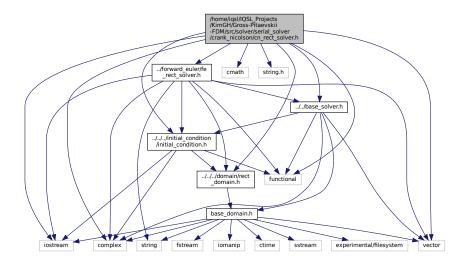
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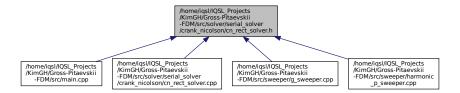
5.19 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/solver/serial_solver/crank_nicolson/cn_rect_solver.h File Reference

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

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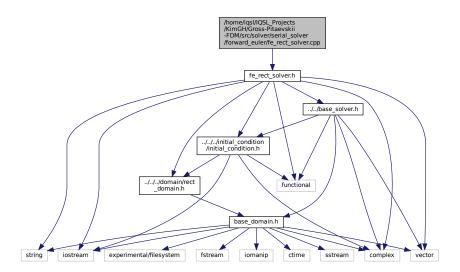
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5.20 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/solver/serial_solver/forward_euler/fe_rect_solver.cpp File Reference

Implementation file for serial forward euler solver methods.

Reference 177

#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

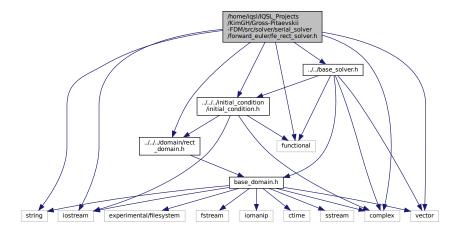
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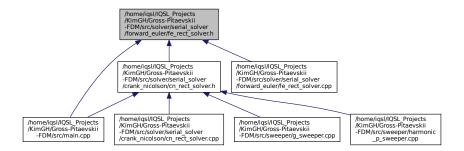
5.21 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/solver/serial_solver/forward_euler/fe_rect_solver.h File Reference

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

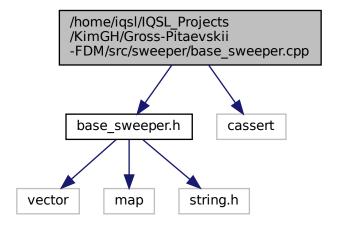
2022-06-05

Copyright

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

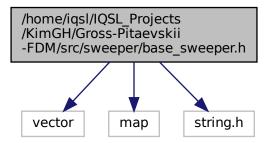
#include "base_sweeper.h"
#include <cassert>
Include dependency graph for base_sweeper.cpp:



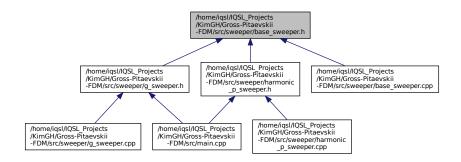
5.23 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/sweeper/base_sweeper.h File Reference

#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

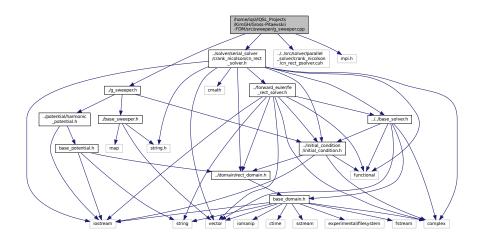
5.24 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/sweeper/g_sweeper.cpp File Reference

```
#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"

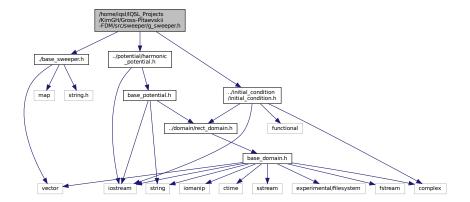
#include <mpi.h>

Include dependency graph for g_sweeper.cpp:

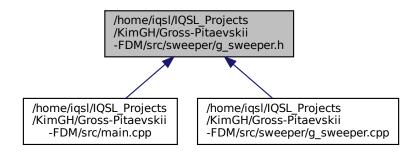


5.25 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/src/sweeper/g_sweeper.h File Reference

```
#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:



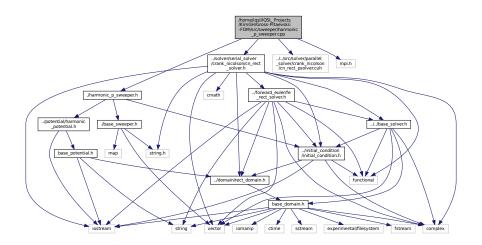
Classes

class GSweeper

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

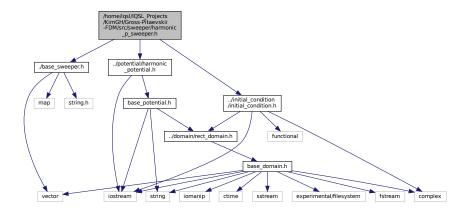
```
#include "./harmonic_p_sweeper.h"
#include "../solver/serial_solver/crank_nicolson/cn_rect_solver.h"
#include "../../src/solver/parallel_solver/crank_nicolson/cn_rect_psolver.
cuh"
#include <mpi.h>
```

Include dependency graph for harmonic_p_sweeper.cpp:

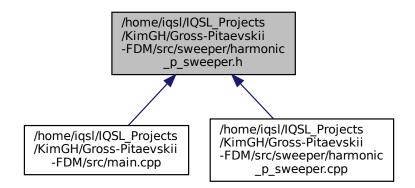


5.27 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD→ M/src/sweeper/harmonic_p_sweeper.h File Reference

```
#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:

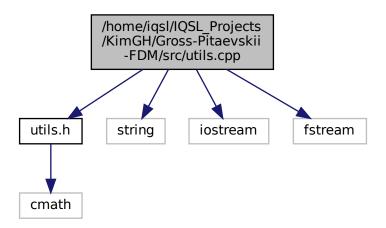


Classes

· class HPSweeper

5.28 /home/iqsl/IQSL_Projects/KimGH/Gross-Pitaevskii-FD M/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

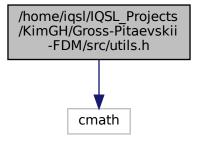
5.28.1.1 is_close()

Definition at line 5 of file utils.cpp.

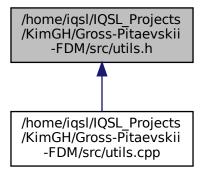
```
5
6 return std::abs(a - b) < tolerance;
7 }
```

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()

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