MOTIONS

Generated by Doxygen 1.8.13

Contents

Chapter 1

MOTIONS - _A Monte Carlo framework for optimal control of plasma_

The program solves optimal control problems governed by the non-linear kinetic equations including external forces and a collision term in a Monte Carlo framwork.

Dependencies and required libraries

The code was optimized for Ubuntu 18.04 LTS. Before downloading the dependencies, make sure that Ubuntu is up-to-date using `sudo apt-get update` and `sudo apt-get upgrade`.

To use the optimizer, `vstrap` must be installed on the machine.

Before compiling the code the following dependencies and libraries must be installed:

- `Armadillo` (this includes lapacke and blas): install using

```
+ openMP: install using
```sudo apt install libomp-de
```

- boost: install using

```
+ build-essentials: install using
+ ```sudo apt-get install build-essentia
```

- cmake: install using

```
For **optional** postprocessing ```python3``` should be installed including the packages
+ argparse
+ pyplot from matplotlib
+ tikzplotlib
+ numpy
+ math
+ pandas

The packages can be installed using the following commands
```sh
sudo apt install python3-pip -y
pip3 install matplotlib tikzplotlib pandas numpy
```

Problem specifications

In the file *Optim_input.xml* it is possible to specify the parameters used by the program. View the comments in te file to get information about the purpose of each parameter. The file `src/controller/optim_controller.cpp` is the core of the optimization.

Structure of the code

The source code is structured in five categories:

- **src/controller**: contains auxiliary subroutines like generating of probability density functions (pdf) and controller for input/output
- **src/io**: contains methods for solving the linear kinetic and adjoint linear kinetic problem
- **src/logger**: core of optimization methods; contains important ncg subroutines and armijo-linesearch as well as functions providing the value of the functional and building the gradient
- **src/objects**: contains python files for visualizing the results of the program
- **src/optimization**:

The program has four more plugins:

- **data**: Here, several test-cases are specified
- **optim-vstrap-toolset**: Imporant plugin for the connection between vstrap and the optimizer
- **pprc**: Files for post-processing (python)
- **test**: gtest files

Compile and run the program

After speficying the parameters, it is possible to compile the code and start the program with the following commands executed in the directory containing the `MOCOKI` folder.

```
mkdir build-Optim && cd build-Optim
cmake ../Optim_VSTRAP
make
./Optim_VSTRAP_CMAKE <path/to/>Optim_input.xml
```

Post-processing

There are `python` files to visualize the results of the MOCOKI code. Assuming the build directory `build-Optim` is at the same directory level as the `Optim_VSTRAP` folder, the following commands executed from the `pprc` folder can be used to visualize data generated by the code.

The following command takes files containing data about development of the value of functional, norm of gradient, norm of control and stepsize during the optimization process and plots these.

```
python3 visualize_control.py ../../data/box_shifting_CSSC/interpolated_control_field.xml
       ../../data/global/box_coarse_512.xml
```

The following command gives plots the control in the current iteration. One has to call the functional specifying the current control and the discretization of the physical domain.

```
python3 post_processing_convergence.py ../../../build-Optim/src/results/
```

Using the dockerized version - UNDER CONSTRUCTION

It is possible to install a docker containing all the needed libraries and dependencies using the following commands executed in the folder in which the `mocoki-image.tar` file is located.

```
sudo docker load < mocoki-image.tar #loads image
sudo docker run --name container_mocoki -it mocoki #creates and starts container named 'container_mocoki'
       using the mocoki:latest image
```

After exiting the container, it can be started again using the command

```
sudo docker container start -ai container_mocoki

Inside the container go inside the ```MOCOKI``` folder and run
```sh
sh setup_cmake.sh
```

This will execute the current version of the code.

You can also change the code outside the docker container and copy it into and from the container using the commands

```
sudo docker cp MOCOKI/ container_mocoki:MOCOKI #copy inside the container
sudo docker cp container_mocoki:build-MOCOKI build-MOCOKI-v08 #copy build folder from container to local
       machine
```

The `sudo` command may be discarded inside docker.
```

Chapter 2

Hierarchical Index

2.1 Class Hierarchy

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

Chapter 3

Class Index

3.1 Class List

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

Chapter 4

Class Documentation

4.1 abstract_controller Class Reference

The abstract_controller class is inherited by all controller classes.

```
#include <abstract_controller.h>
```

Public Member Functions

- data_provider **getData_provider_optim** () const
- void **setData_provider_optim** (const data_provider &value)

4.1.1 Detailed Description

The abstract_controller class is inherited by all controller classes.

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/controller/abstract_controller.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/controller/abstract_controller.cpp

4.2 abstract_verification Class Reference

Public Member Functions

- data_provider **getData_provider_validation** () const
- void **setData_provider_validation** (const data_provider &value)
- data_provider **getData_provider_optim** () const
- void **setData_provider_optim** (const data_provider &value)

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/vldn/controller/abstract_validation.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/vldn/controller/abstract_validation.cpp

4.3 control_field_class.Arrow3D Class Reference

Public Member Functions

- def **__init__** (self, xs, ys, zs, args, kwargs)
- def **draw** (self, renderer)

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/optim-vstrap-toolset/toolset/control_field_class.py

4.4 calculus Class Reference

The calculus class provides method from analysis.

```
#include <calculus.h>
```

Public Member Functions

- double **divergence_vector** (arma::mat input)

Static Public Member Functions

- static std::vector< double > **cross_product** (std::vector< double > v1, std::vector< double > v2)

4.4.1 Detailed Description

The calculus class provides method from analysis.

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/tools/calculus.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/tools/calculus.cpp

4.5 mesh.Cell Class Reference

Public Member Functions

- def **__init__** (self)
- def **set_nodes** (self, nodes)
- def **calc_volume** (self, nodes)
- def **calc_barycenter** (self, nodes)

Public Attributes

- **id**
- **nodes_ids**
- **value**
- **volume**
- **type**
- **barycenter**

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/optim-vstrap-toolset/toolset/mesh.py

4.6 mesh.CellTest Class Reference

Public Member Functions

- def **test_calc_volume** (self)

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/optim-vstrap-toolset/tests/mesh.py

4.7 comparator Class Reference

Public Member Functions

- double **norm_difference_doubleVector** (std::vector< double > v1, std::vector< double > v2)

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/objects/comparator.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/objects/comparator.cpp

4.8 control_field_class.Control_field Class Reference

Public Member Functions

- def **__init__** (self)
- def **__str__** (self)
- def **clear** (self)
- def **create_Lists** (self, controlFile, meshFile, scaling)
- def **plot_Control_field** (self, nodesMesh, endPoints, scaling, directorySRC, boxlim)

Public Attributes

- **control**
- **nodesMesh**
- **endPoints**

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/optim-vstrap-toolset/toolset/control_field_class.py

4.9 control_verification Class Reference

Static Public Member Functions

- static int **start_verification** (int argc, char **argv)
- static std::vector< double > **calculate_mean** (arma::mat control)
- static std::vector< double > **calculate_mean_doubleMatrix** (std::vector< std::vector< double >> control)
- static arma::mat **calculate_cross_error** (arma::mat control, arma::mat barycenters, std::vector< double > &valide_vector)

Additional Inherited Members

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/vldn/control/control_validation.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/vldn/control/control_validation.cpp

4.10 coordinate_phase_space_time Class Reference

The coordinate_phase_space_time class defines coordinates in the seven dimensional time-phase-space cylinder.

```
#include <coordinate_phase_space_time.h>
```

Public Member Functions

- **coordinate_phase_space_time** (int cell_id, int vx, int vy, int vz, int time)
- std::string **toString** () const
- bool operator== (const coordinate_phase_space_time &coordinate) const

  operator == overloads the compare operator. Two objects equal if all attributes equal
- coordinate_phase_space_time **operator-** (const coordinate_phase_space_time &coordinate) const
- int **getPx** () const
- void **setPx** (int value)
- int **getPy** () const
- void **setPy** (int value)
- int **getPz** () const
- void **setPz** (int value)
- int **getVx** () const
- void **setVx** (int value)
- int **getVy** () const
- void **setVy** (int value)
- int **getVz** () const
- void **setVz** (int value)
- int **getTime** () const
- void **setTime** (int value)
- int **getCell_id** () const
- void **setCell_id** (int value)

4.10.1 Detailed Description

The coordinate_phase_space_time class defines coordinates in the seven dimensional time-phase-space cylinder.

4.10.2 Member Function Documentation

4.10.2.1 operator==()

```
bool coordinate_phase_space_time::operator== (
            const coordinate_phase_space_time & coordinate ) const
```

operator == overloads the compare operator. Two objects equal if all attributes equal

Parameters

coordinate	

Returns

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/objects/coordinate_phase_space_time.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/objects/coordinate_phase_space_time.cpp

4.11 data_provider Class Reference

The data_provider class provides the data given in the input file for the optimizer.

```
#include <data_provider.h>
```

Public Member Functions

- **data_provider** (const char *filename)
- std::map< std::string, std::string > **read_paths** (const char *filename)
- std::map< std::string, double > **read_optimization_parameters** (const char *filename)
- std::map< std::string, std::string > **read_subroutines** (const char *filename)
- std::map< int, std::vector< double > > **read_mesh_barycenters** (const char *filename)
- std::map< std::string, std::string > **getPaths** () const
- void **setPaths** (const std::map< std::string, std::string > &value)
- std::map< std::string, double > **getOptimizationParameters** () const
- void **setOptimizationParameters** (const std::map< std::string, double > &value)
- std::map< std::string, std::string > **getSubroutines** () const
- void **setSubroutines** (const std::map< std::string, std::string > &value)
- std::map< int, std::vector< double > > **getMesh_barycenters** () const
- void **setMesh_barycenters** (const std::map< int, std::vector< double > > &value)

Static Public Member Functions

- static arma::mat **convert_barycenters_toArmaMat** (std::map< int, std::vector< double > > barycenters)

4.11.1 Detailed Description

The data_provider class provides the data given in the input file for the optimizer.

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/objects/data_provider.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/objects/data_provider.cpp

4.12 desired_trajectory_controller Class Reference

The desired_trajectory_controller class provides the trajectory of the mean value in phase space.

```
#include <desired_trajectory_controller.h>
```

Public Member Functions

- std::vector< double > trajectory_desired (std::vector< double > barycenter, unsigned int l, unsigned int m, unsigned int n, unsigned int o, std::vector< std::vector< double > > brockettVector, unsigned int plasma_↩ state_output_interval)

  trajectory_desired is the generic function for calling the desired trajectory
- std::vector< double > trajectory_desired_brockett (std::vector< std::vector< double > > brockettVector, unsigned int o, unsigned int plasma_state_output_interval)

  trajectory_desired_brockett provides the desired trajectory using a time dependent vector as input

  –
- std::vector< double > trajectory_desired_parameters (std::vector< double > barycenter, unsigned int l, unsigned int m, unsigned int n, unsigned int o, unsigned int plasma_state_output_interval)

  trajectory_desired_parameters uses the parameters defined in the input file of the optimizer

Public Attributes

- std::map< int, std::vector< double > > **barycenters**

4.12.1 Detailed Description

The desired_trajectory_controller class provides the trajectory of the mean value in phase space.

4.12.2 Member Function Documentation

4.12.2.1 trajectory_desired()

```
std::vector< double > desired_trajectory_controller::trajectory_desired (
            std::vector< double > barycenter,
            unsigned int l,
            unsigned int m,
            unsigned int n,
            unsigned int o,
            std::vector< std::vector< double > > brockettVector,
            unsigned int plasma_state_output_interval )
```

trajectory_desired is the generic function for calling the desired trajectory

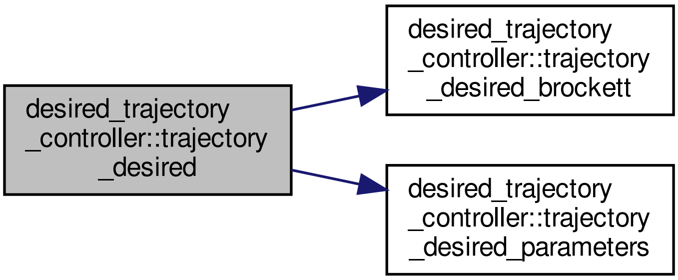
Parameters

barycenter	
l	
m	
n	
o	
brockettVector	
plasma_state_output_interval	

Returns

References trajectory_desired_brockett(), and trajectory_desired_parameters().

Here is the call graph for this function:



4.12.2.2 trajectory_desired_brockett()

```
std::vector< double > desired_trajectory_controller::trajectory_desired_brockett (
            std::vector< std::vector< double > > brockettVector,
            unsigned int o,
            unsigned int plasma_state_output_interval )
```

trajectory_desired_brockett provides the desired trajectory using a time dependent vector as input

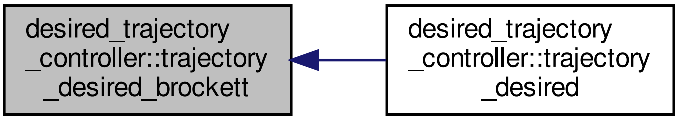
-

Parameters

brockettVector	
o	
plasma_state_output_interval	

Returns

Here is the caller graph for this function:



4.12.2.3 trajectory_desired_parameters()

```
std::vector< double > desired_trajectory_controller::trajectory_desired_parameters (
            std::vector< double > barycenter,
            unsigned int l,
            unsigned int m,
            unsigned int n,
            unsigned int o,
            unsigned int plasma_state_output_interval )
```

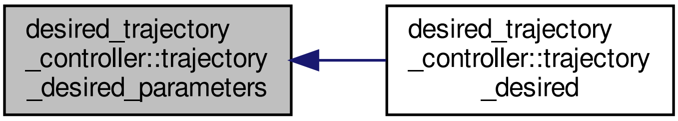
trajectory_desired_parameters uses the parameters defined in the input file of the optimizer

Parameters

barycenter	
l	
m	
n	
o	
plasma_state_output_interval	

Returns

Here is the caller graph for this function:



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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/controller/desired_trajectory_controller.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/controller/desired_trajectory_controller.cpp

4.13 equation_solving_controller Class Reference

Public Member Functions

- int **start_solving_forward** (std::string start_forward)
- int **start_solving_backward** (std::string start_backward)
- arma::mat D1_second_order ()

    D1_second_order calculates the first derivative with respect to position with a seconr oder accuracy (using the Mid-point scheme)
- arma::mat D1_forward ()

    D1_forward calculates the first derivitive with respect to position using the forward scheme (first order accuracy)
- arma::mat D1_backward ()

    D1_backward calculates the first derivitive with respect to position using the backward scheme (first order accuracy)
- arma::mat Laplacian_3D ()

    Laplacian_3D calculates the Laplacion in position in three dimensions.
- arma::mat Laplacian_Squared_3D ()

    Laplacian_Squared_3D.
- arma::mat D1X1_second_order ()
- arma::mat **D1X2_second_order** ()
- arma::mat **D1X3_second_order** ()

4.13.1 Member Function Documentation

4.13.1.1 D1_backward()

```
arma::mat equation_solving_controller::D1_backward ( )
```

D1_backward calculates the first derivitive with respect to position using the backward scheme (first order accuracy)

Returns

4.13.1.2 D1_forward()

```
arma::mat equation_solving_controller::D1_forward ( )
```

D1_forward calculates the first derivitive with respect to position using the forward scheme (first order accuracy)

Returns

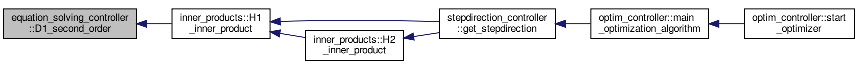
4.13.1.3 D1_second_order()

```
arma::mat equation_solving_controller::D1_second_order ( )
```

D1_second_order calculates the first derivative with respect to position with a seconr oder accuracy (using the Midpoint scheme)

Returns

Here is the caller graph for this function:



4.13.1.4 D1X1_second_order()

```
arma::mat equation_solving_controller::D1X1_second_order ( )
```

for testing

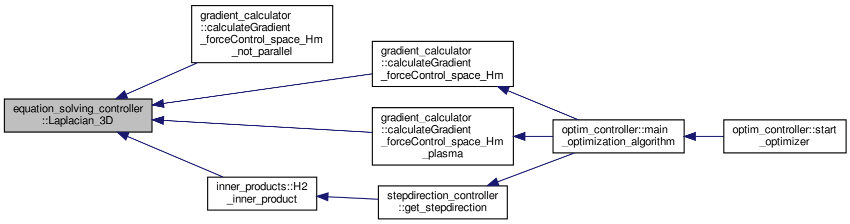
4.13.1.5 Laplacian_3D()

```
arma::mat equation_solving_controller::Laplacian_3D ( )
```

Laplacian_3D calculates the Laplacion in position in three dimensions.

Returns

Here is the caller graph for this function:



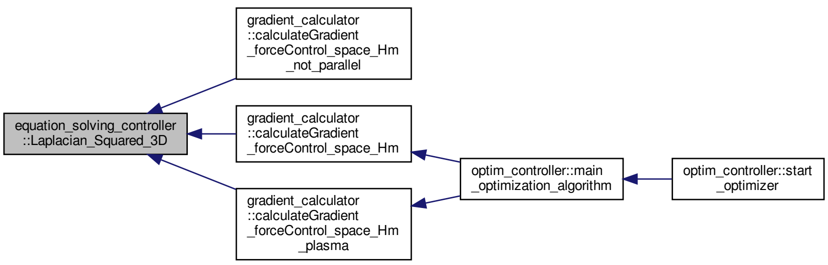
4.13.1.6 Laplacian_Squared_3D()

```
arma::mat equation_solving_controller::Laplacian_Squared_3D ( )
```

Laplacian_Squared_3D.

Returns

Here is the caller graph for this function:



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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/controller/equation_solving_controller.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/controller/equation_solving_controller.cpp

4.14 gradient_calculator Class Reference

The gradient_calculator class provides method for assembling to gradient, which is used in the calculation of the new step-direction for controls in H^2 Sobolev-space For a reference, see https://www.tandfonline.com/doi/abs/10.1080/23324309.2021.1896552.

```
#include <gradient_calculator.h>
```

Public Member Functions

- **gradient_calculator** (const char ∗filename)
- arma::mat calculateGradient_forceControl_space_Hm_not_parallel (std::vector< std::unordered_map< coordinate_phase_space_time, double >> forwardPDF_time, std::vector< std::unordered_map< coordinate_phase_space_time, double >> backwardPDF_time, arma::mat control)

  calculateGradient_forceControl_space_Hm_not_parallel calculates the gradient without using any parallelization;
- arma::mat calculateGradient_forceControl_space_Hm (std::vector< std::unordered_map< coordinate_phase_space_time, double >> forwardPDF_time, std::vector< std::unordered_map< coordinate_phase_space_time, double >> backwardPDF_time, arma::mat control)

  calculateGradient_forceControl_space_Hm calculates the gradient with parallelization
- arma::mat calculateGradient_forceControl_space_Hm_plasma (std::vector< std::unordered_map< coordinate_phase_space_time, double >> forwardPDF_time, std::vector< std::unordered_map< coordinate_phase_space_time, double >> backwardPDF_time, std::vector< std::unordered_map< coordinate_phase_space_time, double >> forwardPDF_time_electrons, std::vector< std::unordered_map< coordinate_phase_space_time, double >> backwardPDF_time_electrons, arma::mat control)

  calculateGradient_forceControl_space_Hm_plasma calculates the gradient with two different species (ions, electrons) present

4.14.1 Detailed Description

The gradient_calculator class provides method for assembling to gradient, which is used in the calculation of the new step-direction for controls in H^2 Sobolev-space For a reference, see https://www.tandfonline.com/doi/abs/10.1080/23324309.2021.1896552.

4.14.2 Member Function Documentation

4.14.2.1 calculateGradient_forceControl_space_Hm()

```
arma::mat gradient_calculator::calculateGradient_forceControl_space_Hm (
            std::vector< std::unordered_map< coordinate_phase_space_time, double >> forwardPDF_time,
            std::vector< std::unordered_map< coordinate_phase_space_time, double >> backwardPDF_time,
            arma::mat control )
```

calculateGradient_forceControl_space_Hm calculates the gradient with parallelization

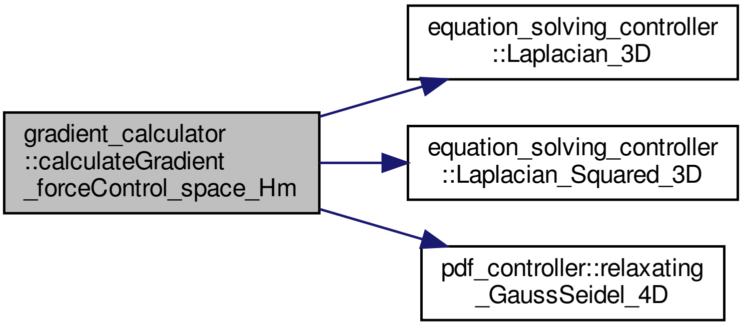
Parameters

forwardPDF_time	
backwardPDF_time	
control	

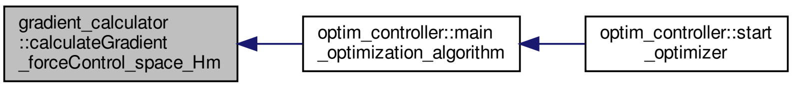
Returns

References equation_solving_controller::Laplacian_3D(), equation_solving_controller::Laplacian_Squared_3D(), and pdf_controller::relaxating_GaussSeidel_4D().

Here is the call graph for this function:



Here is the caller graph for this function:



4.14.2.2 calculateGradient_forceControl_space_Hm_not_parallel()

```
arma::mat gradient_calculator::calculateGradient_forceControl_space_Hm_not_parallel (
            std::vector< std::unordered_map< coordinate_phase_space_time, double >> forward←
PDF_time,
            std::vector< std::unordered_map< coordinate_phase_space_time, double >> backward←
PDF_time,
            arma::mat control )
```

calculateGradient_forceControl_space_Hm_not_parallel calculates the gradient without using any parallelization;

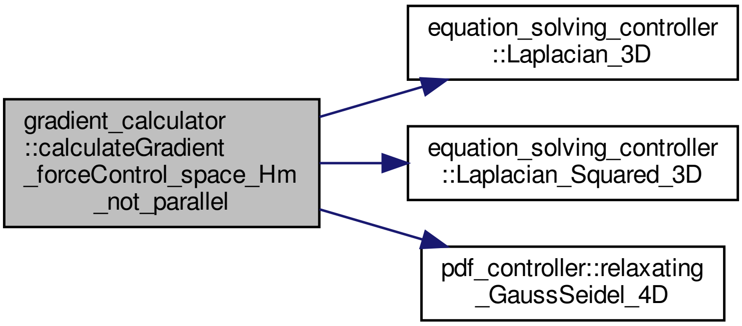
Parameters

forwardPDF_time	
backwardPDF_time	
control	

Returns

References equation_solving_controller::Laplacian_3D(), equation_solving_controller::Laplacian_Squared_3D(), and pdf_controller::relaxating_GaussSeidel_4D().

Here is the call graph for this function:



4.14.2.3 calculateGradient_forceControl_space_Hm_plasma()

```
arma::mat gradient_calculator::calculateGradient_forceControl_space_Hm_plasma (
            std::vector< std::unordered_map< coordinate_phase_space_time, double >> forward←
PDF_time,
            std::vector< std::unordered_map< coordinate_phase_space_time, double >> backward←
PDF_time,
            std::vector< std::unordered_map< coordinate_phase_space_time, double >> forward←
PDF_time_electrons,
            std::vector< std::unordered_map< coordinate_phase_space_time, double >> backward←
PDF_time_electrons,
            arma::mat control )
```

calculateGradient_forceControl_space_Hm_plasma calculates the gradient with two different species (ions, electrons) present

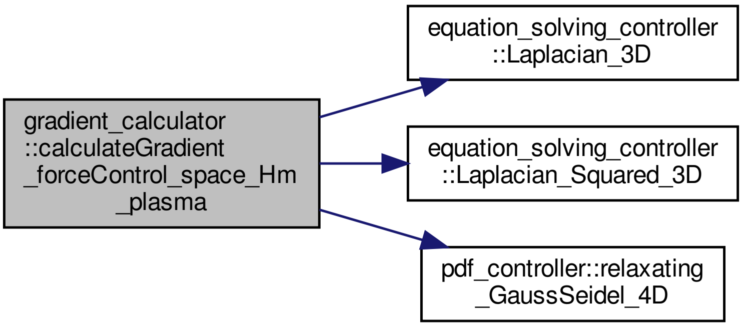
Parameters

forwardPDF_time	
backwardPDF_time	
forwardPDF_time_electrons	
backwardPDF_time_electrons	
control	

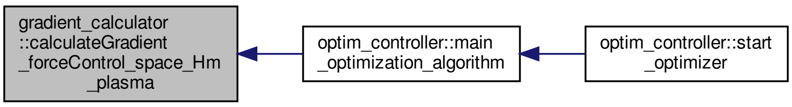
Returns

References equation_solving_controller::Laplacian_3D(), equation_solving_controller::Laplacian_Squared_3D(), and pdf_controller::relaxating_GaussSeidel_4D().

Here is the call graph for this function:



Here is the caller graph for this function:



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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/optimization/gradient_calculator.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/optimization/gradient_calculator.cpp

4.15 gradient_validation Class Reference

Static Public Member Functions

- static int **landau_validation** (int argc, char **argv)

Additional Inherited Members

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/vldn/gradient/gradient_validation.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/vldn/gradient/gradient_validation.cpp

4.16 std::hash< coordinate_phase_space_time > Struct Template Reference

Public Types

- typedef coordinate_phase_space_time **argument_type**
- typedef size_t **result_type**

Public Member Functions

- size_t **operator()** (const argument_type &x) const

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/objects/coordinate_phase_space_time.h

4.17 inner_products Class Reference

Public Member Functions

- double **L2_inner_product** (arma::mat m1, arma::mat m2)
- double H1_inner_product (arma::mat m1, arma::mat m2)
- double H2_inner_product (arma::mat m1, arma::mat m2)

4.17.1 Member Function Documentation

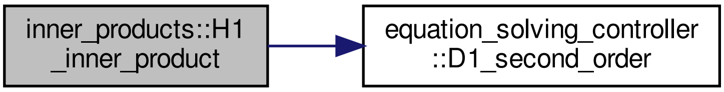
4.17.1.1 H1_inner_product()

```
double inner_products::H1_inner_product (
            arma::mat m1,
            arma::mat m2 )
```

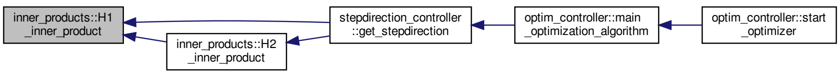
L2 part

References equation_solving_controller::D1_second_order().

Here is the call graph for this function:



Here is the caller graph for this function:



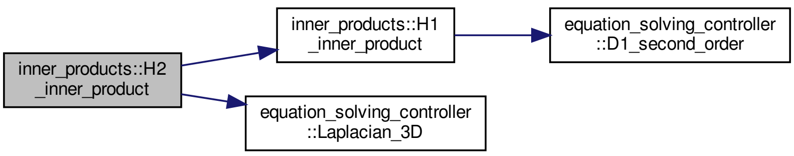
4.17.1.2 H2_inner_product()

```
double inner_products::H2_inner_product (
            arma::mat m1,
            arma::mat m2 )
```

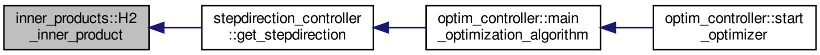
L2 and H1 part

References H1_inner_product(), and equation_solving_controller::Laplacian_3D().

Here is the call graph for this function:



Here is the caller graph for this function:



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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/tools/inner_products.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/tools/inner_products.cpp

4.18 input Class Reference

Public Member Functions

- unsigned int **read_plasma_state_forward** (std::vector< std::vector< particle >> &forwardParticles, std::string file_name)
- unsigned int **read_plasma_state_backward** (std::vector< std::vector< particle >> &backwardParticles, std::string file_name)
- arma::mat readControl (const char *filename, int number_cells_position)

    readControl reads in control cells (control in volume, xml format)

Static Public Member Functions

- static std::vector< particle > **readParticleVector** (std::string filename, std::string delimiter)
- static std::vector< std::vector< double > > **readDoubleMatrix** (std::string filename, int number_cells_position, std::string delimiter)
- static std::vector< double > **readDoubleVector** (const char *filename)
- static std::vector< std::vector< double > > readBrockettFile (std::string filename, std::string delimiter, unsigned int lines)

    readBrockettFile reads file with time-dependent desired trajectory of the mean

4.18.1 Member Function Documentation

4.18.1.1 readBrockettFile()

```
std::vector< std::vector< double > > input::readBrockettFile (
            std::string filename,
            std::string delimiter,
            unsigned int lines ) [static]
```

readBrockettFile reads file with time-dependent desired trajectory of the mean

Parameters

filename	
delimiter	
lines	

Returns

4.18.1.2 readControl()

```
arma::mat input::readControl (
            const char * filename,
            int number_cells_position )
```

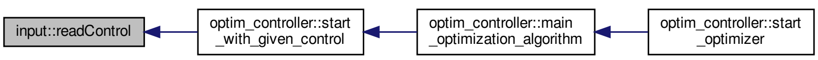
readControl reads in control cells (control in volume, xml format)

Parameters

filename	
number_cells_position	

Returns

Here is the caller graph for this function:



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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/io/input.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/io/input.cpp

4.19 mesh.Mesh Class Reference

Public Member Functions

- def **__init__** (self)

- def **__str__** (self)
- def **clear** (self)
- def **read_mesh_xml** (self, file_name)
- def **interpolate_cell2node** (self)
- def **read_control_csv** (self, file_name)
- def **read_control_xml** (self, file_name)
- def **write_control_csv** (self, file_name)
- def **write_control_xml** (self, file_name, control_type)
- def **write_barycenters_xml** (self, file_name)

Public Attributes

- **cells**
- **nodes**
- **volume**

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/optim-vstrap-toolset/toolset/mesh.py

4.20 mesh.MeshTest Class Reference

Public Member Functions

- def **test_read_mesh_xml** (self)
- def **test_read_control_csv** (self)
- def **test_read_control_xml** (self)
- def **test_interpolate_cell2node** (self)

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/optim-vstrap-toolset/tests/mesh.py

4.21 mesh.Node Class Reference

Public Member Functions

- def **__init__** (self, id=0, coord=(0.0, 0.0, 0.0))
- def **get_position** (self)

Public Attributes

- **id**
- **x_coord**
- **y_coord**
- **z_coord**
- **value**

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/optim-vstrap-toolset/toolset/mesh.py

4.22 objective_calculator Class Reference

The objective_calculator class calculates the objective/functional according to Brockett's approach of ensemble optimal control problems; see, e.g., Bartsch, J., Borzì, A., Fanelli, F. et al. A theoretical investigation of Brockett's ensemble optimal control problems. Calc. Var. 58, 162 (2019). https://doi.org/10.↩ 1007/s00526-019-1604-2.

`#include <objective_calculator.h>`

Public Member Functions

- **objective_calculator** (const char ∗filename)
- double **calculate_objective** (std::vector< std::unordered_map< coordinate_phase_space_time, double >> forwardPDF_time, arma::mat control)

4.22.1 Detailed Description

The objective_calculator class calculates the objective/functional according to Brockett's approach of ensemble optimal control problems; see, e.g., Bartsch, J., Borzì, A., Fanelli, F. et al. A theoretical investigation of Brockett's ensemble optimal control problems. Calc. Var. 58, 162 (2019). https://doi.org/10.↩ 1007/s00526-019-1604-2.

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/optimization/objective_calculator.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/optimization/objective_calculator.cpp

4.23 optim_controller Class Reference

The optim_controller class provides methods for starting and the optimizer and visualizing the results.

`#include <optim_controller.h>`

Public Member Functions

- int start_optimizer (int argc, const char ∗∗argv)

  start_optimizer reads in the command line command and starts the optimizer

Static Public Member Functions

- static int main_optimization_algorithm (const char ∗input_xml_path)

  main_optimization_algorithm is the core optimization algorithm which uses the paramteres defined in the input file for the optimizer
- static arma::mat start_with_zero_control (const char ∗input_xml_path)

  start_with_zero_control deletes the whole folder containing the files from the last optimization run, creates a new initial guess that is zero everywhere
- static arma::mat start_with_given_control (const char ∗input_xml_path)

  start_with_given_control delets only the txt and csv files and starts with the control that is currently in the results folder
- static int generate_input_files (const char ∗input_xml_path)

  generate_input_files starts the generation of the VSTRAP input files for forward, backward and adjoint_creation
- static int post_processing_convergence (data_provider provider)

  post_processing_convergence starts the python post-processing method
- static int visualize_control (data_provider provider)

  visualize_control starts the python method for visualizing the control in three dimensions
- static int paraview_plot_forward (data_provider provider)

  paraview_plot_forward starts the python routine for displaying the evolution of the solution to the forward equation using a python script for paraview

4.23.1 Detailed Description

The optim_controller class provides methods for starting and the optimizer and visualizing the results.

4.23.2 Member Function Documentation

4.23.2.1 generate_input_files()

```
int optim_controller::generate_input_files (
            const char * input_xml_path )  [static]
```

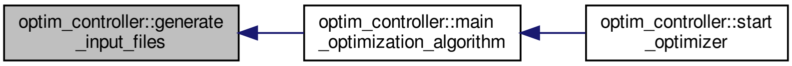
generate_input_files starts the generation of the VSTRAP input files for forward, backward and adjoint_creation

Parameters

input_xml_path	

Returns

Here is the caller graph for this function:



4.23.2.2 main_optimization_algorithm()

```
int optim_controller::main_optimization_algorithm (
            const char * input_xml_path )  [static]
```

main_optimization_algorithm is the core optimization algorithm which uses the paramteres defined in the input file for the optimizer

Parameters

input_xml_path	

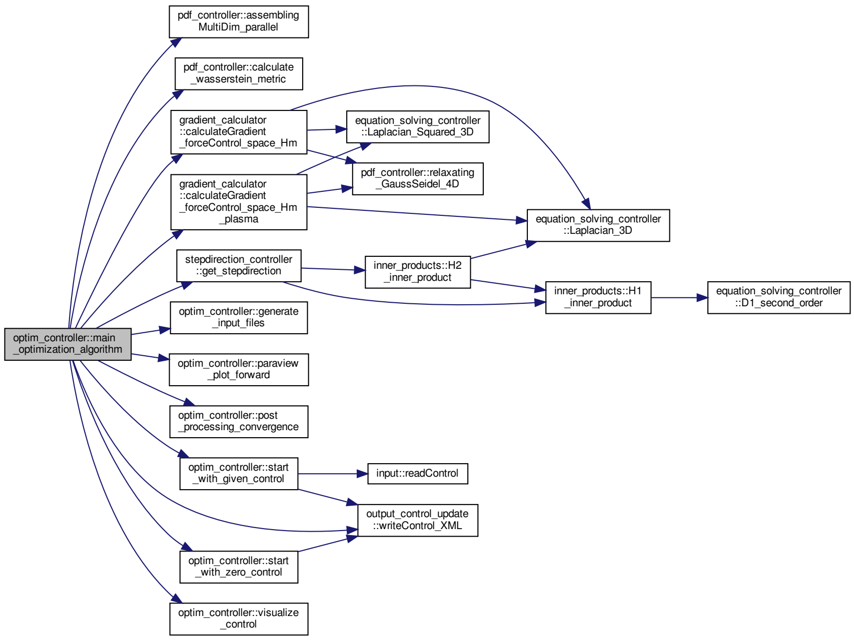
Returns

START OPTIMIZATION ITERATION

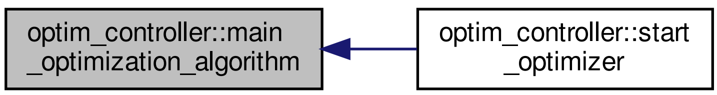
first stepsize guess, scaled with norm of gradient

References pdf_controller::assemblingMultiDim_parallel(), pdf_controller::calculate_wasserstein_metric(), gradient_calculator::calculateGradient_forceControl_space_Hm(), gradient_calculator::calculateGradient_forceControl_space_Hm_plasma(), generate_input_files(), stepdirection_controller::get_stepdirection(), paraview_plot_forward(), post_processing_convergence(), start_with_given_control(), start_with_zero_control(), visualize_control(), and output_control_update::writeControl_XML().

Here is the call graph for this function:



Here is the caller graph for this function:



4.23.2.3 paraview_plot_forward()

```
int optim_controller::paraview_plot_forward (
            data_provider provider )  [static]
```

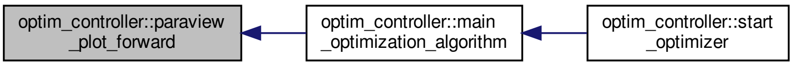
paraview_plot_forward starts the python routine for displaying the evolution of the solution to the forward equation using a python script for paraview

Parameters

provider	

Returns

Here is the caller graph for this function:



4.23.2.4 post_processing_convergence()

```
int optim_controller::post_processing_convergence (
            data_provider provider )  [static]
```

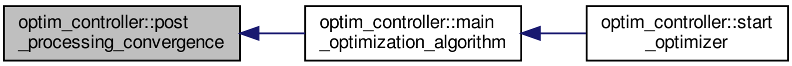
post_processing_convergence starts the python post-processing method

Parameters

provider	

Returns

Here is the caller graph for this function:



4.23.2.5 start_optimizer()

```
int optim_controller::start_optimizer (
            int argc,
            const char ** argv )
```

start_optimizer reads in the command line command and starts the optimizer

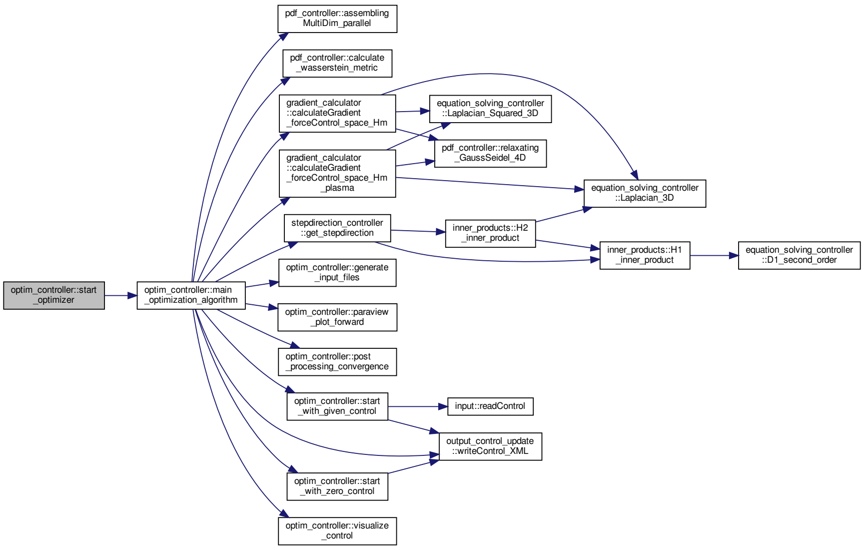
Parameters

argc	
argv	

Returns

References main_optimization_algorithm().

Here is the call graph for this function:



4.23.2.6 start_with_given_control()

```
arma::mat optim_controller::start_with_given_control (
            const char * input_xml_path )  [static]
```

start_with_given_control delets only the txt and csv files and starts with the control that is currently in the results folder

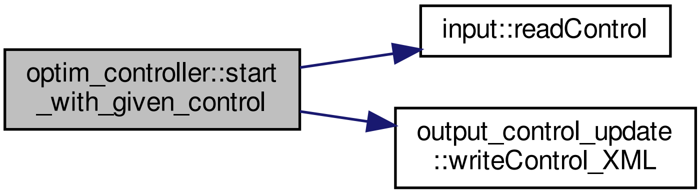
Parameters

input_xml_path	

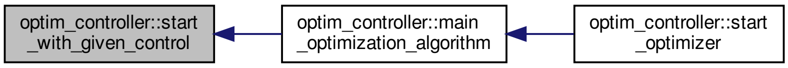
Returns

References input::readControl(), and output_control_update::writeControl_XML().

Here is the call graph for this function:



Here is the caller graph for this function:



4.23.2.7 start_with_zero_control()

```
arma::mat optim_controller::start_with_zero_control (
            const char * input_xml_path )  [static]
```

start_with_zero_control deletes the whole folder containing the files from the last optimization run, creates a new initial guess that is zero everywhere

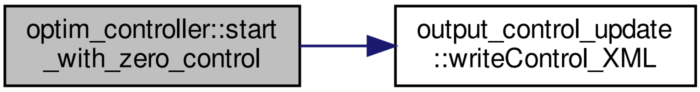
Parameters

input_xml_path	

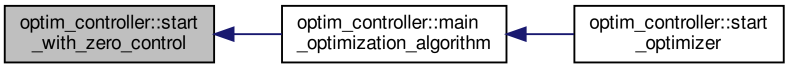
Returns

References output_control_update::writeControl_XML().

Here is the call graph for this function:



Here is the caller graph for this function:



4.23.2.8 visualize_control()

```
int optim_controller::visualize_control (
            data_provider provider )  [static]
```

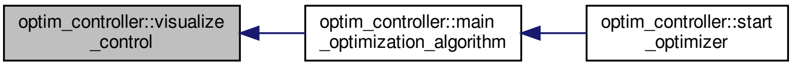
visualize_control starts the python method for visualizing the control in three dimensions

Parameters

provider	

Returns

Here is the caller graph for this function:



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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/controller/optim_controller.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/controller/optim_controller.cpp

4.24 output_control_update Class Reference

The output_control_update class offers functions to write the update of the control in a file that is readable by the solver for forward and backward equation.

```
#include <output_control_update.h>
```

Public Member Functions

- **output_control_update** (const char ∗filename)
- int writeControl_XML (arma::mat control)

  writeControl_XML takes a control and writes a corresponding XML file

Static Public Member Functions

- static int **interpolate_control** (data_provider provider)

4.24.1 Detailed Description

The output_control_update class offers functions to write the update of the control in a file that is readable by the solver for forward and backward equation.

4.24.2 Member Function Documentation

4.24.2.1 writeControl_XML()

```
int output_control_update::writeControl_XML (
            arma::mat control )
```

writeControl_XML takes a control and writes a corresponding XML file

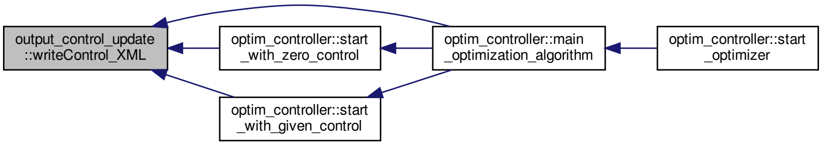
Parameters

control	(arma::mat)

Returns

0 if processed successfully

Here is the caller graph for this function:



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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/io/output_control_update.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/io/output_control_update.cpp

4.25 output_diagnostics Class Reference

The output_diagnostics class writes the value of different objects to txt files.

```
#include <output_diagnostics.h>
```

Public Member Functions

- int **writeGradientMatrixToFile** (arma::mat gradient, std::string filename)
- int **writeArmaMatrixToFile** (arma::mat input, std::string filename)
- int **writeDoubleToFile** (double value, std::string filename)
- int **writeDoubleVectorToFile** (std::vector< double > vector, std::string filename)

4.25.1 Detailed Description

The output_diagnostics class writes the value of different objects to txt files.

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/io/output_diagnostics.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/io/output_diagnostics.cpp

4.26 parameter_sanity Class Reference

The parameter_sanity class provides sanity checks for parameters definied in the input file of the optimizer.

```
#include <parameter_sanity.h>
```

Public Member Functions

- int **check_adjoint_velocity** (data_provider provider)
- int **check_velocity_discretization** (data_provider provider)

4.26.1 Detailed Description

The parameter_sanity class provides sanity checks for parameters definied in the input file of the optimizer.

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/tools/parameter_sanity.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/tools/parameter_sanity.cpp

4.27 particle Class Reference

The particle class defines a particle using its position, velocity and weight.

```
#include <particle.h>
```

Public Member Functions

- **particle** (double vx, double vy, double vz)
- **particle** (double px, double py, double pz, double vx, double vy, double vz)
- **particle** (double px, double py, double pz, double vx, double vy, double vz, int cell_id)
- bool operator== (const particle &particle) const

  operator == overloads the compare operator. Two particles equal if the difference of the values in every component is less than a given tolerance (comparing two doubles)
- double getVelocityMagnitudeParticle ()

  getVelocityMagnitudeParticle calculates speed of particles using Euclidean Norm
- std::string **toString** ()
- double **getPx** () const
- void **setPx** (double value)
- double **getPy** () const
- void **setPy** (double value)
- double **getPz** () const
- void **setPz** (double value)
- double **getVx** () const
- void **setVx** (double value)
- double **getVy** () const
- void **setVy** (double value)
- double **getVz** () const
- void **setVz** (double value)
- int **getCell_id** () const
- void **setCell_id** (int value)
- double **getWeight** () const
- void **setWeight** (double value)

4.27.1 Detailed Description

The particle class defines a particle using its position, velocity and weight.

4.27.2 Member Function Documentation

4.27.2.1 getVelocityMagnitudeParticle()

```
double particle::getVelocityMagnitudeParticle ( )
```

getVelocityMagnitudeParticle calculates speed of particles using Euclidean Norm

Returns

4.27.2.2 operator==()

```
bool particle::operator== (
            const particle & particle ) const
```

operator == overloads the compare operator. Two particles equal if the difference of the values in every component is less than a given tolerance (comparing two doubles)

Parameters

particle	

Returns

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/objects/particle.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/objects/particle.cpp

4.28 pdf_controller Class Reference

The pdf_controller class provides important method for assembling and smoothing of probability density functions (pdfs)

```
#include <pdf_controller.h>
```

Public Member Functions

- int assemblingMultiDim (std::vector< std::vector< particle > > &particlesTime, unsigned int equationType, std::vector< std::unordered_map< coordinate_phase_space_time, double > > &pdf_time)

  assemblingMultiDim performs the assembling of the probability density distribution from the particles vector in phase-time-space
- int assemblingMultiDim_parallel (std::vector< std::vector< particle > > &particlesTime, unsigned int equationType, std::vector< std::unordered_map< coordinate_phase_space_time, double > > &pdf_time)

  assemblingMultiDim_parallel performs the assembling of the probability density distribution from the particles vector in phase-time-space in parallel
- std::vector< std::vector< std::vector< std::vector< double > > > > relaxating_GaussSeidel_4D (std↩ ::vector< std::vector< std::vector< std::vector< double > > > > pdf, unsigned int numberOfRelaxation↩ Steps)

  relaxating_GaussSeidel_4D relaxes/smoothes the probability distribution according to denoising techniques using partial differential equations (`https://ieeexplore.ieee.org/document/6175261`*) and the the GaussSeidel algorithm This is important for calculating the derivative with respect to velocity in the gradient.*
- double calculate_wasserstein_metric (std::vector< std::vector< particle > > dist1, std::vector< std::vector< particle > > dist2)
- double **calculate_wasserstein_metric_histogramm** (std::vector< std::unordered_map< coordinate_↩ phase_space_time, double > > dist1, std::vector< std::unordered_map< coordinate_phase_space_time, double > > dist2)

4.28.1 Detailed Description

The pdf_controller class provides important method for assembling and smoothing of probability density functions (pdfs)

4.28.2 Member Function Documentation

4.28.2.1 assemblingMultiDim()

```
int pdf_controller::assemblingMultiDim (
            std::vector< std::vector< particle > > & particlesTime,
            unsigned int equationType,
            std::vector< std::unordered_map< coordinate_phase_space_time, double > > & pdf↩
_time )
```

assemblingMultiDim performs the assembling of the probability density distribution from the particles vector in phase-time-space

Parameters

particlesTime	
equationType	
pdf_time	

Returns

4.28.2.2 assemblingMultiDim_parallel()

```
int pdf_controller::assemblingMultiDim_parallel (
            std::vector< std::vector< particle > > & particlesTime,
            unsigned int equationType,
            std::vector< std::unordered_map< coordinate_phase_space_time, double > > & pdf←
_time )
```

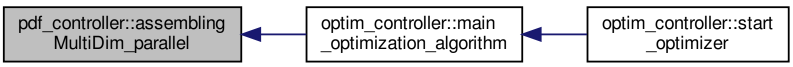
assemblingMultiDim_parallel performs the assembling of the probability density distribution from the particles vector in phase-time-space in parallel

Parameters

particlesTime	
equationType	
pdf_time	

Returns

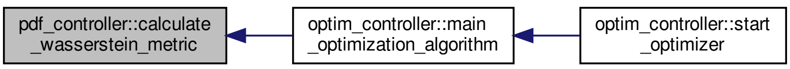
Here is the caller graph for this function:



4.28.2.3 calculate_wasserstein_metric()

```
double pdf_controller::calculate_wasserstein_metric (
            std::vector< std::vector< particle > > dist1,
            std::vector< std::vector< particle > > dist2 )
```

currently not used Here is the caller graph for this function:



4.28.2.4 relaxating_GaussSeidel_4D()

```
std::vector< std::vector< std::vector< std::vector< double > > > > pdf_controller::relaxating↩
_GaussSeidel_4D (
            std::vector< std::vector< std::vector< std::vector< double > > > > pdf,
            unsigned int numberOfRelaxationSteps )
```

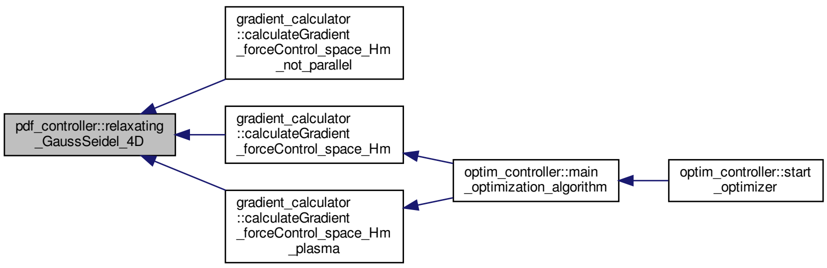
relaxating_GaussSeidel_4D relaxes/smoothes the probability distribution according to denoising techniques using partial differential equations (https://ieeexplore.ieee.org/document/6175261) and the the GaussSeidel algorithm This is important for calculating the derivative with respect to velocity in the gradient.

Parameters

pdf	
numberOfRelaxationSteps	

Returns

Here is the caller graph for this function:



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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/controller/pdf_controller.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/controller/pdf_controller.cpp

4.29 stepdirection_controller Class Reference

The stepdirection_controller class provides different methods for finding the step-direction, as gradient descent and non-linear conjugate gradient (NCG) schemes with different update rules; see e.g. https://www.caam.↩ rice.edu/~yzhang/caam554/pdf/cgsurvey.pdf.

```
#include <stepdirection_controller.h>
```

Public Member Functions

- **stepdirection_controller** (const char ∗filename)
- arma::mat get_stepdirection (arma::mat gradient, arma::mat gradient_old, arma::mat stepdirectionOld, unsigned int optimization_iteration)

  get_stepdirection is a generic method called in the main optimizer algorithm

4.29.1 Detailed Description

The stepdirection_controller class provides different methods for finding the step-direction, as gradient descent and non-linear conjugate gradient (NCG) schemes with different update rules; see e.g. https://www.caam.rice.edu/~yzhang/caam554/pdf/cgsurvey.pdf.

4.29.2 Member Function Documentation

4.29.2.1 get_stepdirection()

```
arma::mat stepdirection_controller::get_stepdirection (
            arma::mat gradient,
            arma::mat gradient_old,
            arma::mat stepdirectionOld,
            unsigned int optimization_iteration )
```

get_stepdirection is a generic method called in the main optimizer algorithm

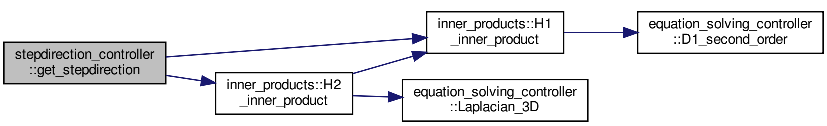
Parameters

gradient	
gradient_old	
stepdirectionOld	
optimization_iteration	

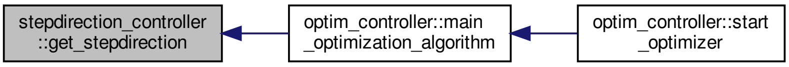
Returns

References inner_products::H1_inner_product(), and inner_products::H2_inner_product().

Here is the call graph for this function:



Here is the caller graph for this function:



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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/optimization/stepdirection_controller.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/optimization/stepdirection_controller.cpp

4.30 stepsize_controller Class Reference

The stepsize_controller class provides different methods for finding an accepted step-size (resulting in a decreasing value of the functional)

```
#include <stepsize_controller.h>
```

Public Member Functions

- **stepsize_controller** (const char ∗filename)
- int **calculate_stepsize** (arma::mat &gradient, double J0, arma::mat &control, arma::mat &stepdirection, std::vector< particle > &inputParticles, double &stepsize0)

4.30.1 Detailed Description

The stepsize_controller class provides different methods for finding an accepted step-size (resulting in a decreasing value of the functional)

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

- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/optimization/stepsize_controller.h
- /home/jan/Promotion_linuxPC/Optim_VSTRAP/src/optimization/stepsize_controller.cpp