Optim\_VSTRAP

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### **Chapter 1**

# LARA - \_A Monte Car\*\*L\*\*o framework for optim\*\*A\*\*I cont\*\*R\*\*ol of plasm\*\*A\*\*\_

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  $src/controller/optim\_controller. \leftarrow cpp$  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  $build-\leftarrow Optim$  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.

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.

```
\verb|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.

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.

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# **Chapter 2**

# **Hierarchical Index**

### 2.1 Class Hierarchy

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

abstract_controller
calculus
comparator
desired_trajectory_controller
equation_solving_controller
gradient_calculator
inner_products
input
objective_calculator
optim_controller
output_control_update
output_diagnostics
pdf_controller
stepdirection_controller
stepsize_controller
abstract_verification
control verification
gradient_validation
mesh.Cell
control_field_class.Control_field
coordinate phase space time
data_provider
std::hash< coordinate phase space time >
mesh.Mesh
mesh.Node
parameter_sanity
particle
TestCase
mesh.CellTest
mesh.MeshTest
FancyArrowPatch
control_field_class.Arrow3D

6 Hierarchical Index

# **Chapter 3**

# **Class Index**

#### 3.1 Class List

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

abstract_controller	
The abstract_controller class is inherited by all controller classes	9
abstract_verification	11
control_field_class.Arrow3D	12
calculus	
Method from analysis	12
mesh.Cell	14
mesh.CellTest	14
comparator	15
control_field_class.Control_field	16
control_verification	16
coordinate_phase_space_time	
Defines coordinates in the seven dimensional time-phase-space cylinder	17
data_provider	18
desired_trajectory_controller	
The desired_trajectory_controller class provides the trajectory of the mean value in phase space	18
1 = 0=	20
gradient_calculator	
Method for assembling to gradient, which is used in the calculation of the new step-direction for	
controls in $H^{\wedge}$ 2 Sobolev-space	21
<b>3</b> ··· · · ⊆ ·· · · · · · ·	24
	25
<del></del>	25
	27
	29
mesh.MeshTest	29
	30
objective_calculator	
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.←	
	31
·	32
output_control_update	
Offers functions to write the update of the control in a file that is readable by the solver for forward	
	~ 4

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putput_diagnostics	
Writes the value of different objects to txt files	36
parameter_sanity	
Sanity checks for parameters definied in the input file of the optimizer	37
particle	38
odf_controller	39
stepdirection_controller	
Different methods for finding the step-direction, as gradient descent and NCG schemes with	
different update rules	40
stepsize_controller	
Different methods for finding an accepted step-size (resulting in a decreasing value of the func-	
tional)	42

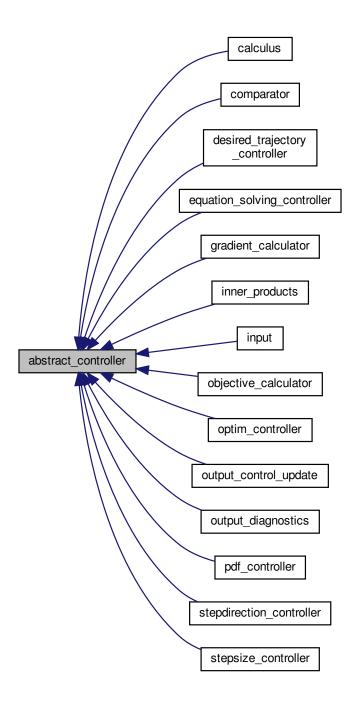
# **Chapter 4**

# **Class Documentation**

4.1 abstract\_controller Class Reference

The abstract\_controller class is inherited by all controller classes.

Inheritance diagram for abstract\_controller:



#### **Public Member Functions**

- data\_provider getData\_provider\_optim () const
- void setData\_provider\_optim (const data\_provider &value)

#### 4.1.1 Detailed Description

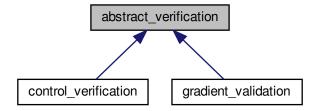
The abstract\_controller class is inherited by all controller classes.

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

Inheritance diagram for abstract\_verification:



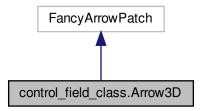
#### **Public Member Functions**

- 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)

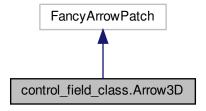
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/vldn/controller/abstract\_validation.h
- $\bullet \ \ / home/jan/Promotion\_linuxPC/Optim\_VSTRAP/vldn/controller/abstract\_validation.cpp$

#### 4.3 control\_field\_class.Arrow3D Class Reference

Inheritance diagram for control\_field\_class.Arrow3D:



Collaboration diagram for control\_field\_class.Arrow3D:



#### **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:

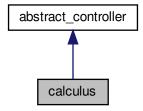
• /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/optim-vstrap-toolset/control\_field\_class.py

#### 4.4 calculus Class Reference

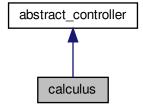
The calculus class provides method from analysis.

#include <calculus.h>

Inheritance diagram for calculus:



Collaboration diagram for calculus:



#### **Public Member Functions**

• double divergence\_vector (arma::mat input)

#### **Static Public Member Functions**

 $\bullet \quad \text{static std::vector} < \text{double} > \textbf{cross\_product} \ (\text{std::vector} < \text{double} > \text{v1}, \ \text{std::vector} < \text{double} > \text{v2}) \\$ 

#### 4.4.1 Detailed Description

The calculus class provides method from analysis.

- $\bullet \ \ / home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/tools/calculus.h$
- /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**

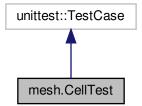
- id
- · nodes\_ids
- value
- volume
- type
- barycenter

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

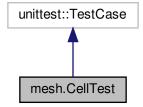
• /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/optim-vstrap-toolset/toolset/mesh.py

#### 4.6 mesh.CellTest Class Reference

Inheritance diagram for mesh.CellTest:



Collaboration diagram for mesh.CellTest:



**Public Member Functions** 

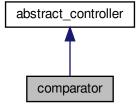
• def test\_calc\_volume (self)

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

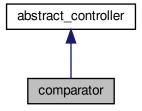
• /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/optim-vstrap-toolset/tests/mesh.py

#### 4.7 comparator Class Reference

Inheritance diagram for comparator:



Collaboration diagram for comparator:



**Public Member Functions** 

• double norm\_difference\_doubleVector (std::vector< double > v1, std::vector< double > v2)

- /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**

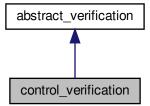
- · control
- nodesMesh
- · endPoints

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

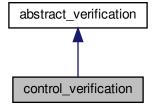
/home/jan/Promotion\_linuxPC/Optim\_VSTRAP/optim-vstrap-toolset/toolset/control\_field\_class.py

#### 4.9 control\_verification Class Reference

Inheritance diagram for control\_verification:



Collaboration diagram for control verification:



#### Static Public Member Functions

- static int start\_verification (int argc, char \*\*argv)
- static 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\_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
- 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.

- /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

#### **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)

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

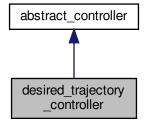
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/objects/data\_provider.h
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/objects/data\_provider.cpp

#### 4.12 desired\_trajectory\_controller Class Reference

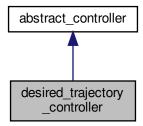
The desired\_trajectory\_controller class provides the trajectory of the mean value in phase space.

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

Inheritance diagram for desired\_trajectory\_controller:



Collaboration diagram for desired\_trajectory\_controller:



#### **Public Member Functions**

- std::vector< double > trajectory\_desired (std::vector< double > barycenter, unsigned int I, unsigned int m, unsigned int n, unsigned int o, std::vector< std::vector< double > > brockettVector, unsigned int plasma\_
   state\_output\_interval)
- 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

#### 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\_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	
0	
plasma_state_output_interval	

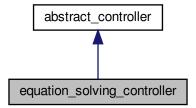
Returns

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

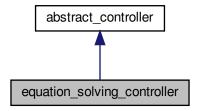
- $\bullet \ \ / home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/controller/desired\_trajectory\_controller.h$
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/controller/desired\_trajectory\_controller.cpp

### 4.13 equation\_solving\_controller Class Reference

Inheritance diagram for equation\_solving\_controller:



Collaboration diagram for equation\_solving\_controller:



#### **Public Member Functions**

- int start\_solving\_forward (std::string start\_forward)
- int start\_solving\_backward (std::string start\_backward)
- arma::mat D1\_second\_order ()
- · arma::mat D1\_forward ()
- arma::mat D1\_backward ()

- arma::mat Laplacian\_3D ()
- arma::mat Laplacian\_Squared\_3D ()
- arma::mat D1X1\_second\_order ()
- arma::mat D1X2\_second\_order ()
- arma::mat D1X3\_second\_order ()

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

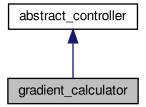
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/controller/equation\_solving\_controller.h
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/controller/equation\_solving\_controller.cpp

#### 4.14 gradient\_calculator Class Reference

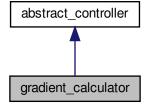
The gradient\_calculator class provides method for assembling to gradient, which is used in the calculation of the new step-direction for controls in  $H^2$  Sobolev-space.

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

Inheritance diagram for gradient\_calculator:



Collaboration diagram for gradient\_calculator:



#### **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.

#### 4.14.2 Member Function Documentation

#### 4.14.2.1 calculateGradient\_forceControl\_space\_Hm()

calculateGradient forceControl space Hm calculates the gradient with parallelization

#### **Parameters**

forwardPDF_time	
backwardPDF_time	
control	

#### Returns

#### 4.14.2.2 calculateGradient\_forceControl\_space\_Hm\_not\_parallel()

calculateGradient\_forceControl\_space\_Hm\_not\_parallel calculates the gradient without using any parallelization;

#### **Parameters**

forwardPDF_time	
backwardPDF_time	
control	

#### Returns

#### 4.14.2.3 calculateGradient\_forceControl\_space\_Hm\_plasma()

calculateGradient\_forceControl\_space\_Hm\_plasma calculates the gradient with two different species (ions, electrons) present

#### **Parameters**

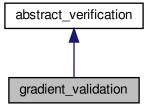
forwardPDF_time	
backwardPDF_time	
forwardPDF_time_electrons	
backwardPDF_time_electrons	
control	

#### Returns

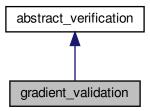
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/optimization/gradient\_calculator.h
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/optimization/gradient\_calculator.cpp

#### 4.15 gradient\_validation Class Reference

Inheritance diagram for gradient\_validation:



Collaboration diagram for gradient\_validation:



#### **Static Public Member Functions**

• static int landau\_validation (int argc, char \*\*argv)

#### **Additional Inherited Members**

- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/vldn/gradient/gradient\_validation.h
- $\bullet \ \ / home/jan/Promotion\_linuxPC/Optim\_VSTRAP/vldn/gradient/gradient\_validation.cpp$

#### 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**

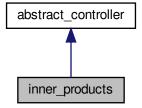
• size\_t operator() (const argument\_type &x) const

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

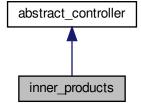
• /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/objects/coordinate\_phase\_space\_time.h

#### 4.17 inner\_products Class Reference

Inheritance diagram for inner\_products:



Collaboration diagram for inner\_products:



#### **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()

L2 part

#### 4.17.1.2 H2\_inner\_product()

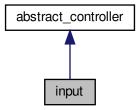
L2 and H1 partHere is the call graph for this function:

```
inner_products::H2 ____inner_product = __inner_product
```

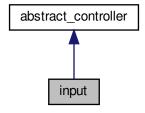
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/tools/inner\_products.h
- $\bullet \ \ /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/tools/inner\_products.cpp$

#### 4.18 input Class Reference

Inheritance diagram for input:



Collaboration diagram for input:



#### **Public Member Functions**

- unsigned int read\_plasma\_state\_backward (std::vector< std::vector< particle >> &backwardParticles, std::string file\_name)
- arma::mat readControl (const char \*filename, int pcell\_gp)

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 pcell\_gp, 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()

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

#### **Parameters**

filename	
pcell_gp	

#### Returns

- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/io/input.h
- $\bullet \ \ /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/io/input.cpp$

#### 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**

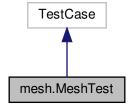
- · cells
- nodes
- volume

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

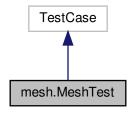
• /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/optim-vstrap-toolset/toolset/mesh.py

#### 4.20 mesh.MeshTest Class Reference

Inheritance diagram for mesh.MeshTest:



Collaboration diagram for mesh.MeshTest:



#### **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:

 $\bullet \ \ / home/jan/Promotion\_linuxPC/Optim\_VSTRAP/optim-vstrap-toolset/tests/mesh.py$ 

#### 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:

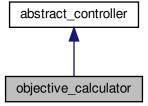
 $\bullet \ \ / home/jan/Promotion\_linuxPC/Optim\_VSTRAP/optim-vstrap-toolset/toolset/mesh.py$ 

# 4.22 objective\_calculator Class Reference

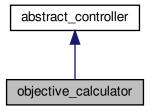
The objective\_calculator class calculates the objective/functional according to Brockett's approach of ensemble optimal control problems; see, e.g., Bartsch, J., Borzì, A., Fanelli, F. et al. A theoretical investigation of Brockett's ensemble optimal control problems. Calc. Var. 58, 162 (2019). https://doi.org/10.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

#include <objective\_calculator.h>

Inheritance diagram for objective\_calculator:



Collaboration diagram for objective\_calculator:



### **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

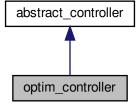
The objective\_calculator class calculates the objective/functional according to Brockett's approach of ensemble optimal control problems; see, e.g., Bartsch, J., Borzì, A., Fanelli, F. et al. A theoretical investigation of Brockett's ensemble optimal control problems. Calc. Var. 58, 162 (2019). https://doi.org/10.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

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

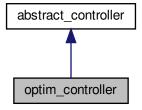
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/optimization/objective\_calculator.h
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/optimization/objective\_calculator.cpp

# 4.23 optim\_controller Class Reference

Inheritance diagram for optim\_controller:



Collaboration diagram for optim\_controller:



# **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

# 4.23.1 Member Function Documentation

# 4.23.1.1 main\_optimization\_algorithm()

main\_optimization\_algorithm is the core optimization algorithm which uses the paramteres defined in the input file for the optimizer

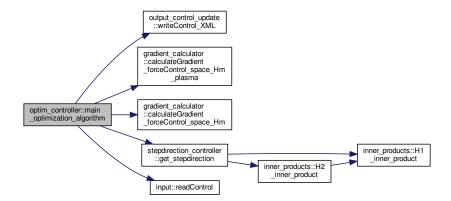
### **Parameters**

input\_xml\_path

Returns

# START OPTIMIZATION ITERATION

first stepsize guess, scaled with norm of gradientHere is the call graph for this function:



### 4.23.1.2 start\_optimizer()

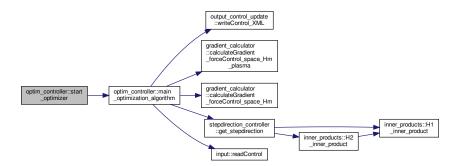
start\_optimizer reads in the command line command and starts the optimizer

### **Parameters**

argc	
argv	

# Returns

Here is the call graph for this function:



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

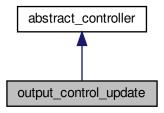
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/controller/optim\_controller.h
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/controller/optim\_controller.cpp

# 4.24 output\_control\_update Class Reference

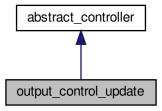
The output\_control\_update class offers functions to write the update of the control in a file that is readable by the solver for forward and backward equation.

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

Inheritance diagram for output\_control\_update:



Collaboration diagram for output\_control\_update:



# **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
- int writeArmaMatrixToFile (arma::mat input, std::string filename)

### **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()

writeControl XML takes a control and writes a corresponding XML file

#### **Parameters**

```
control (arma::mat)
```

### Returns

0 if processed successfully

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

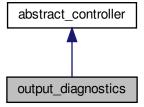
- $\bullet \ \ / home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/io/output\_control\_update.h$
- $\bullet \ \ / home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/io/output\_control\_update.cpp$

# 4.25 output\_diagnostics Class Reference

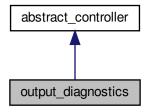
The output\_diagnostics class writes the value of different objects to txt files.

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

Inheritance diagram for output diagnostics:



Collaboration diagram for output\_diagnostics:



#### **Public Member Functions**

- int writeArmaMatrixToFile (arma::mat gradient, 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
- $\bullet \ \ /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/tools/parameter\_sanity.cpp$

# 4.27 particle Class Reference

# **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
- double getVelocityMagnitudeParticle ()

getVelocityMagnitudeParticle calculates speed of particles using Euclidean Norm

• std::string toString ()

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 Member Function Documentation

### 4.27.1.1 getVelocityMagnitudeParticle()

 $\label{thm:double_particle::getVelocityMagnitudeParticle ()} \end{substitute}$ 

getVelocityMagnitudeParticle calculates speed of particles using Euclidean Norm

Returns

# 4.27.1.2 toString()

```
std::string particle::toString ( )
```

toString

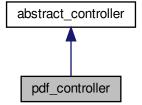
Returns

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

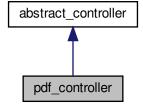
- $\bullet \ \ / home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/objects/particle.h$
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/objects/particle.cpp

# 4.28 pdf\_controller Class Reference

Inheritance diagram for pdf\_controller:



Collaboration diagram for pdf\_controller:



### **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)

- int assemblingMultiDim\_parallel (std::vector< std::vector< particle > > &particlesTime, unsigned int equationType, std::vector< std::unordered\_map< coordinate\_phase\_space\_time, double > > &pdf\_time)
- 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)

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

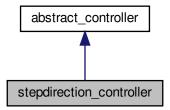
- /home/jan/Promotion linuxPC/Optim VSTRAP/src/controller/pdf controller.h
- /home/jan/Promotion linuxPC/Optim VSTRAP/src/controller/pdf controller.cpp

# 4.29 stepdirection controller Class Reference

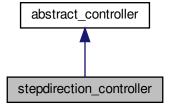
The <u>stepdirection\_controller</u> class provides different methods for finding the step-direction, as gradient descent and NCG schemes with different update rules.

#include <stepdirection\_controller.h>

Inheritance diagram for stepdirection\_controller:



Collaboration diagram for stepdirection controller:



# **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 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 NCG schemes with different update rules.

#### 4.29.2 Member Function Documentation

### 4.29.2.1 get\_stepdirection()

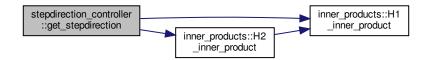
get\_stepdirection generic method called in the main optimizer algorithm

# Parameters

gradient	
gradient_old	
stepdirectionOld	
optimization_iteration	

#### Returns

Here is the call graph for this function:



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

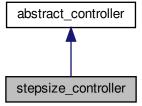
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/optimization/stepdirection\_controller.h
- /home/jan/Promotion\_linuxPC/Optim\_VSTRAP/src/optimization/stepdirection\_controller.cpp

# 4.30 stepsize\_controller Class Reference

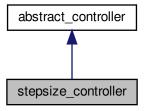
The stepsize\_controller class provides different methods for finding an accepted step-size (resulting in a decreasing value of the functional)

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

Inheritance diagram for stepsize\_controller:



Collaboration diagram for stepsize\_controller:



# **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