Appendix A: user manual for the particle method library

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1 Building and running the example program with Hodgkin-Huxley model

1.1 Structure of the repository

This repository contains the source code for the method, in the form of a C++ library, that consists of particle_method.h and particle_method.cpp, as well as an example program, which serves as a suggestion on how the library can be used. The example can be viewed by opening the minimal_HH_mat_example.sln solution file. The code is written using C++, and the example program is built on a Windows machine using Microsoft Visual studio 2019. The instruction will be based on this environment though the principle for building this program on other platform is similar. Since this program uses external libraries, some patience is needed in setting the program to work.

1.2 Required external libraries

The list of required libraries are listed according the specific header and source file loaded.

• particle_method.h and particle_method.cpp

There are two options for building these files. If macro MATLAB_VISUALIZE is enabled, then matlab is required, and libeng.lib;libmx.lib;libmat.lib; are library files needed to be added at Linker-Input-Additional dependencies in the project property pages. Please refer to this page from mathworks website for further instruction. Additionally, the system environment MATLAB should be set to the matlab root folder.

Alternatively, when real-time visualization is not required and the use of a large program is not preferred, the HDF5 serves as an alternative data input output library. We recommend using vcpkg to setup HDF5 library in visual studio. The following command

```
vcpkg install hdf5[cpp]:x64-windows ---recurse
```

would download this package. Be warned that hdf5 and matlab have conflicting dll files, and it is important to check which dll file is loaded at runtime. If vcpkg is not used, then zlib.lib;hdf5.lib;hdf5_cpp.lib needed to be added at Linker→Input→Additional dependencies

Independent of the two options, intel-tbb is required for parallel computing. Additionally, boost and Eigen are libraries required. The following command

```
vcpkg install tbb:x64-windows --recurse
vcpkg install boost[boost-odeint]:x64-windows
vcpkg install boost[boost-ublas]:x64-windows
vcpkg install boost[boost-program-options]:x64-windows
vcpkg install eigen3:x64-windows
```

would set these libraries. If vcpkg is not used, tbb.lib needs to be added to Linker→Input→Additional dependencies.

• minimal_XX_neuron_example.cpp

The boost-program-options is needed to compile this file. If vcpkg is not used, then the correct version of libboost_program_options needs to be added to Linker-Input-Additional dependencies.

• set_XX_eqns.h This header file does not require additional library to build.

1.3 Building the program

The projects in the solution are set to use the matlab version out-of-box. The program should build with one click if the external libraries are correctly set.

1.4 Common issues and solution

- LNK2001 at build time. Likely due to libraries not setup correctly, which may occur either when library is missing, or different versions of the same library exist. Using vcpkg would reduce the chance of this happening than manually tracing each library.
- undefined reference to some_function at xx.dll at run time. In addition to the common cause of not properly setting the correct version of matlab, this is also likely to be caused by a conflict in dll file. HDF5 and matlab both comes with hdf5.dll, however they are not interchangeable. To make sure the correct dll is loaded, check if hdf5.dll exist in current directory or the Windows\System32 directory. Then, the order of the directories stored in system PATH variable would determine which hdf5.dll will be used.

1.5 Running the example program

The program uses boost::program_options to parse options, and help info can be accessed using the -h option:

```
| Second | S
```

Figure 1: Help message produced by the program

By default, the program will not produce any visual output as -i (--plot_interval) = 0, and the only output files are HHTestatend.mat, which stores the end condition of the system as a linear combination of particles, and coupling_strength_diff_X_coup_Y.mat, which logs the coupling strength, averaged membrane potential, and particle count through the process.

Using the -i %d option will generate a visualization that looks as follows:

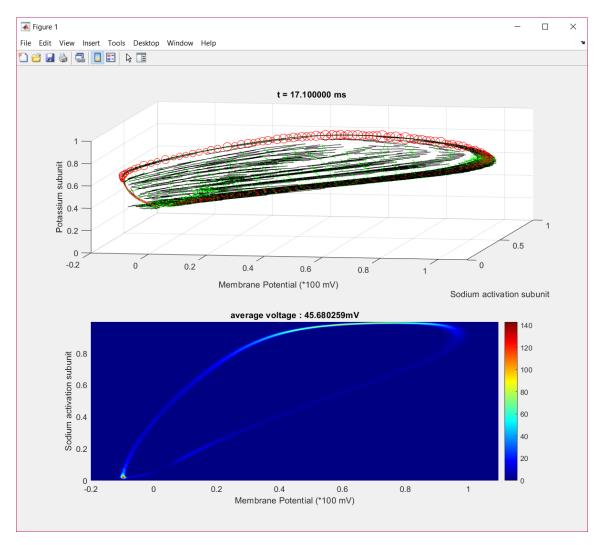


Figure 2: A screenshot of the visualization

Note that the plots, especially the density heat map is computationally intensive, and will significantly slow down the program.

1.6 Program options in the example program

- -d --diffusion_coeff Changes the diffusion coefficient. The diffusion coefficient is set to be isotropic in this example program.
- --tol Tolerance for the linear approximation, as relative error, before a particle needs to be split. Increasing tolerance decreases the number of particles, however it can lead to inaccurate results.

- -s --stepsize Maximum step size for the adaptive time step differential equation solver. Increasing time step may lead to slower computation time as additional split of particles may be introduced during each time step.
- -p --projection_dimension Index of dimensions to project to in the scatter plot of population density. The projection can be onto a 1,2, or 3 dimensional subspace. The index starts at 0
- -q --density_projection_dimension Index of dimensions to project to in the density plot of population density. The projection can be onto a 1 or 2 dimensional subspace. The index starts at 0.
- -v --video Generates a video of all plots drawn during the duration of the simulation. Please note that in matlab 2019b or later versions, the default save location for the video is the folder where the matlab executable file is located, instead of the folder where this example program is located. To change the behavior, use cd command in matlab to change the output path to the desired location.

2 Adapting the program to different problems

The example program is called *minimal* in the sense that only the most common parameters can be adjusted at run time, whereas the model and other parameters are determined at compile time, in order to present a short example. To adapt the program to a different model, the following areas needs to be considered:

2.1 Modifying models and parameters

In the example project, the models are contained in the set_hh_eqns.h and set_SAN_eqns.h for the Hodgkin-Huxley and Simplified averaged neuron model respectively. To set a model, a custom struct Advection_diffusion_eqn with the following properties needs to be defined:

Additionally, if state_variable_always_valid is false, then the following properties are also required:

```
vector_bool_function state_variable_in_domain;//Returns true if the variable is ←
   inside the domain.
vector_vector_function state_variable_restrict_to_domain;//A method that maps ←
   particles out of domain back inside. (Such particles can be produced when ←
   particles are splitted.)
//Note: Since a lambda function cannot change value of input
```

The following are two examples of struct Advection_diffusion_eqn.

The first example is the 2-dimensional Van der Pol oscillator with that is coupled by the average value in the first variable:

```
{\tt Advection\_diffusion\_eqn* set\_van\_der\_pol\_eqn(const value\_type diffusion\_coeff) } \ \{ (const value\_type diffusion\_coeff) \} \ \{ (const value\_type diffusion\_coeff) \} \ \{ (const value\_type diffusion\_coeff) \} \} \ \{ (const value\_type diffusion\_coeff) \} \ \{ (const value\_type diffusion\_coeff) \} \} \ \{ (const value\_type diffusion\_coeff) \} \ \{ (const value\_type diffusion\_coeff) \} \} \ \{ (const value\_type diffusion\_coeff) \} \ \{ (const value\_type diffusion\_coeff) \} \} \ \{ (const value\_type diffusion\_coeff) \} \ \{ (const value\_type diffusion\_coeff) \} \} \ \{ (const value\_type diffusion\_coeff) \} \ \{ (const value\_type diffusion\_coeff) \} \} \ \{ (const value\_type diffusion\_coeff) \} \ \{ (const value\_type diffusion\_coeff) \} \} \ \{ (const value\_type diffusion\_coeff) \} \ \{ (const value\_type diffusion\_coeff) \} \} \ \{ (const value\_type diffusion\_coeff) \} \ \{ (const value\_type diffusion\_coeff) \} \} \ \{ (const value\_type diffusion\_coeff) \} \} \ \{ (const value\_type diffusion\_coeff) \} \ \{ (const va
       dimensional state space with an overloaded diffusion coefficient that is \hookleftarrow
               symmetric in each direction (i.e. diffusion coefficient matrix is identity ↔
                matrix multiplied by scalar diffusion coefficient), and the state variable \leftrightarrow
               domain is the whole space
       {\tt vector\_function\ advection\_dynamics;\ // declares\ dynamics\ as\ a\ vector\_valued\ } \leftarrow
                function
        coupling\_velocity\_function coupling\_velocity; // declares coupling velocity function (\hookleftarrow
                see example below
        {\tt coupling\_strength\_function} \ \ {\tt coupling\_strength}; // \ {\tt declares} \ \ {\tt coupling} \ \ {\tt strength} \ \ {\tt function} \ \ (\hookleftarrow
                       example below
       //advection_dynamics is defined as the following lambda-function that returns the \hookleftarrow
               time derivative dxdt given the state variable x:
       advection_dynamics = [](const State_variable& x) {
               value\_type mu = 1.5;
               State_variable dxdt(2);
               \}; //A coupling velocity function takes input x as the state variable of the POST-\leftrightarrow
               synaptic oscillator, which given the vector-valued coupling_strength, will have \leftarrow its time derivative modified by dxdt:
       coupling_velocity = [](const State_variable& x, const value_type coupling_strength) ←
               State_variable dxdt(2);
               \begin{array}{lll} \texttt{dxdt} \, [\, 0\, ] &=& \texttt{coupling\_strength} \, ; \\ \texttt{dxdt} \, [\, 1\, ] &=& 0\,.0 \, ; \end{array}
               return dxdt; //In this example, the dxdt is given by coupling_strength in the ↔
                       first coordinate.
       }; //A coupling strength function computes the coupling strength output from a PRE\leftrightarrow
               synaptic oscillator given its state in the current and a previous state, as \leftarrow well as the time difference between these two states.
       \texttt{coupling\_strength} = \texttt{[](const~Particle\&~current\_state~,~const~Particle\&~prev\_state~,~} \leftarrow
               const value_type delta_t) {
               //NOTE: coupling strength should compute some average flow rate over the \leftrightarrow time_step period, NOT the instantaneous flow rate at a given time.
               //The choice is made to avoid computing coupling strength on a derivative
                //which would be very sensitive to choice of timestep, and may miss some firing \leftrightarrow
               when time_step is too large.

//For an "averaged value type" coupling as shown here, this is not a big issue, ←

but it does not hurt to compute average of the two.
               {\tt const} value_type coupling_coefficient = 0.5;
               * coupling_coefficient * current_state.weight;//returns the average value
                       in coordinate 1(defined by center_location) weighted with a coupling \leftarrow
                       coefficient and the weight of this particle.
       };
//NOTE: state_variable_in_domain and state_variable_restrict_to_domain not required ↔
               since state variable is valid everywhere.
        //defines the return value using pointers. Due to constraint of C++, defining an \leftrightarrow
               incomplete class is only possible using pointers.
       eqn_ptr->advection_velocity = advection_dynamics;
       \verb|eqn_ptr->| \verb|coupling_velocity| = \verb|coupling_velocity|;
       eqn_ptr->coupling_strength = coupling_strength;
       return eqn_ptr;
```

In the following example, the Hodgkin-Huxley equation with a threshold-type coupling is defined. It is copied from set_hh_eqn.h with additional comment:

```
\texttt{Advection\_diffusion\_eqn*} \hspace{0.2cm} \texttt{set\_Hodgkin\_Huxley\_eqn(const} \hspace{0.2cm} \texttt{value\_type} \hspace{0.2cm} \texttt{diffusion\_coeff} \hspace{0.2cm}, \hspace{0.2cm} \texttt{const} \hspace{0.2cm} \hookleftarrow \hspace{0.2cm} \texttt{onst} \hspace{0.2cm} \hookleftarrow \hspace{0.2cm} \texttt{onst} \hspace{0.2cm} \longleftrightarrow \hspace{0.2cm} 
            value_type coupling_strength_coefficient, const value_type coupling_potential) {
          auto eqn_ptr = new Advection_diffusion_eqn(4, diffusion_coeff, false);//defines a 4
                      dimensional state space with an overloaded diffusion coefficient that is ↔
                      symmetric in each direction (i.e. diffusion coefficient matrix is identity ←
                      matrix multiplied by scalar diffusion coefficient), and the state variable \leftarrow domain is restrained. (With restriction defined later)
           vector_vector_function advection_dynamics;
           coupling_velocity_function coupling_velocity;
          coupling_strength_function coupling_strength;
//definition of a standard HH model:
          advection_dynamics = [](const State_variable& x) {
    //x[0] = V / 100; rest ordered by M, N, H.
    const value_type gna = 120;
    const value_type ena = 115; const value_type gk = 36;
                      const value_type ek = -12;
                      const value_type gl = 0.3;
                      const value_type el = 10.613;
                      const value_type appcurr = 8.0;
                      State_variable dxdt(4U);
                      const value_type M = x[1];
                      const value_type N = x[2];
                      const value_type H = x[3];
                      const value\_type Ah = 0.07*exp(-V / 20.0);
                      //function y = Am(V)
                      const value_type Am = (25.0 - V) / (10.0*(exp((25.0 - V) / 10.0) - 1.0));
                      //function y = An(V)
                      const value_type An = (10.0 - V) / (100.0*(exp((10.0 - V) / 10.0) - 1.0));
                      // function y = Bh(V)
                      const value_type Bh = 1.0 / (exp((30.0 - V) / 10.0) + 1.0);
                      // function y = Bm(V)
                      const value_type Bm = 4.0*exp(-V / 18.0);
                      // function y = Bn(V)
                      const value_type Bn = 0.125*exp(-V / 80.0);
                      //%Bn = 0.125*exp(-V / 19.7); //this is for the Corrected HH model dxdt[1] = Am * (1 - M) - Bm * M; dxdt[2] = An * (1 - N) - Bn * N; dxdt[3] = Ah * (1 - H) - Bh * H;
                      //std::cout << dxdt;
                       return dxdt:
           //definition of coupling strength, given PRE-synaptic oscillator particle at current↔
                         state and a previous state that was coupling_time_step ago:
           \texttt{coupling\_strength} = [\texttt{coupling\_strength\_coefficient}] (\texttt{const} \ \texttt{Particle\&} \ \texttt{current\_state} \ , \ \hookleftarrow
                      const Particle& prev_state, const value_type coupling_time_step) {
                      //NOTE: coupling strength should compute the average flow rate over the
                      coupling_time_step period, NOT the instantaneous flow rate at a given time. //The choice is made to avoid computing coupling strength on a derivative,
                      //which would be very sensitive to choice of timestep, and may miss some firing \leftrightarrow
                      when coupling_time_step is too large.
//For a "Threshold type" coupling, this means the value should be divided by ↔
                                 coupling_time_step
                      {\tt const} value_type threshold_voltage = 0.45;// threshold voltage of 45 mV
                       \begin{tabular}{ll} \textbf{if} & (\texttt{current\_state.center\_location} \, [\,0\,] \end{tabular} <= \begin{tabular}{ll} \texttt{prev\_state.center\_location} \, [\,0\,] \end{tabular} 
                                  //No coupling when the membrane potential is decreasing.
                                 return 0.0;
                      //The following 3 lines compute the proportion (of the whole population) of the \leftrightarrow
                                population crossing the threshold voltage:
                      \overline{\text{const}} value_type V_normalized = (current_state.center_location[0] - \leftrightarrow
                                \texttt{threshold\_voltage}) \ / \ \mathsf{sqrt} \big( \mathsf{current\_state.covariance\_matrix} \big( 0 \,, 0 \big) \, \big) \, ;
                      {\tt const} \ \ {\tt value\_type} \ \ {\tt V\_prev\_normalized} \ = \ ({\tt prev\_state.center\_location} \ [0] \ - \ \hookleftarrow
                                 \texttt{threshold\_voltage}) \ / \ \texttt{sqrt} \big( \texttt{prev\_state.covariance\_matrix} \big( 0 \,, \ 0 \big) \, \big) \, ;
```

```
const value_type population_proportion = (erf(V_normalized / sqrt(2)) - erf(<math>\leftrightarrow
          V_{prev_normalized} / sqrt(2)) * 0.5;
     //Which is further adjusted by the coupling_strength_coefficient and weighr of \leftrightarrow
          particle, and divided by the time step since the coupling is computed as a \leftarrow velocity term, and should not be scaled by the choice of coupling time step\leftarrow
     return population_proportion * coupling_strength_coefficient / ↔
          coupling_time_step * current_state.weight;
const value_type coupling_potential_rescaled = coupling_potential / 100.0;
//The coupling velocity defines how the POST-synaptic particle is affected, which in ↔ this particular example is a conductance-based coupling model:
\texttt{coupling\_velocity} = [\texttt{coupling\_potential\_rescaled}] (\texttt{const} \ \texttt{State\_variable\&} \ \texttt{target} \ , \ \longleftrightarrow \\
     \begin{array}{ll} \textbf{const} & \texttt{value\_type} & \texttt{coupling\_strength} ) & \{ \\ //dV/dt & = k \left( V\_c - V \right) \end{array}
     State_variable rval(target.size());
     rval.fill(0.0);
     \verb|rval[0]| = \verb|coupling_strength| * (\verb|coupling_potential_rescaled| - target[0]);
     return rval:
};
//Since HH model has 3 variables restricted between 0 and 1, the following function \leftrightarrow
     that determines if a coordinate is inside the domain is REQUIRED:
{\tt vector\_bool\_function\ state\_variable\_in\_domain}\ ;
\tt state\_variable\_in\_domain = [](const\ State\_variable\ x)\ \{
     1.0)
          return false;
     return true;
}; //Additionally, a function to restrict such coordinates back to domain is also \leftrightarrow
vector_vector_function state_variable_restrict_to_domain;
state_variable_restrict_to_domain = [](State_variable x) {
     auto x_copy = x;
if (x_copy[1] < 0.0)
    x_copy[1] = 0.0;</pre>
     else if (x_copy[1] >
                               1.0)
     x_{copy}[1] = 1.0;
if (x_{copy}[2] < 0.0)
x_{copy}[2] = 0.0;
     else if (x_copy[2] > 1.0)
     x_{copy}[2] = 1.0;
if (x_{copy}[3] < 0.0)
          x_{copy}[3] = 0.0;
     else if (x_copy[3] >
         x_{copy}[3] = 1.0;
     return x_copy;
 /define return value:
eqn_ptr->advection_velocity = advection_dynamics;
eqn_ptr->coupling_strength = coupling_strength;
eqn_ptr->coupling_velocity = coupling_velocity;
eqn_ptr->state_variable_in_domain = state_variable_in_domain;
eqn_ptr->state_variable_restrict_to_domain = state_variable_restrict_to_domain;
return eqn_ptr;
```

2.2 Modifying procedural source file

After changing the model files, additional parameters independent from the model (such as timestep, total timestep count, and scalar parameters) needs modification as well. The procedural setup of the model in main and related functions also needs to be adjusted accordingly. How the desired parameters can be introduced is a generic programming problem and is beyond the scope here.

However, we remind readers that:

- Inside run_HH_model, make sure that the dimension are set correctly
- The plot parameters used here are specific to the chosen Hodgkin-Huxley model here

2.3 Modifying initial condition

The initial condition is defined by a mat file with following variables:

```
%d-dimensional state variable, with initial condition as a linear combination of n ↔ particles:
w_array%1* n matrix, defines weight of each particle
x_array%d*n matrix, defines center location of each particle
sigma_array%d*d*n matrix, defines covariance of each particle
```

Note since mat uses column-major while hdf5 uses row-major, the h5 files will have reversed dimension ordering. An initial condition in h5 file is defined as follows:

```
//d-dimensional state variable, with initial condition as a linear combination of n ↔ particles:
x_array//n*d matrix of 64-bit floating-point
w_array//n*1 matrix of 64-bit floating-point
sigma_array//n*d*d matrix of 64-bit floating-point
```

3 Usage for individual functions in particle_method.h

This section documents the usage of the functions and objects defined in particle_method.h.

- #define MATLAB_VISUALIZE: defines if the matlab version or hdf5 version of data input/output should be used.
- Vector and Matrix-valued variables are defined as Eigen vectors and matrices. specifically:

```
typedef Eigen::VectorXd State_variable;
typedef Eigen::MatrixXd Matrix_type;
typedef double value_type;
typedef int index_type;
```

• Mathematical functions are defined using the lambda functions implemented using the C++ standard library. Specifically:

```
typedef std::function<State_variable(const State_variable)> vector_vector_function ← ;
typedef std::function<value_type(const State_variable)> vector_scalar_function;
typedef std::function<br/>
typedef std::function<void(const State_variable)> vector_bool_function;
typedef std::function<void(State_variable)> vector_void_function;
```

• struct Particle An asymmetric particle.

– member variables

```
State_variable center_location;
Matrix_type covariance_matrix;
value_type weight;
```

constructor

two initializing methods:

- helper functions:

method to find density values at a location in the state space:

```
value_type density_at(const State_variable& location) const;
```

Find density for marginal distribution where only a subset of coordinates in the location input is considered:

```
value_type density_projection_at_coordinate(const State_variable& location, \hookleftarrow const std::vector<br/>
bool>& range_dimensions) const;//range_dimensions is of \hookleftarrow length dimension. e.g. TFTF means projection to dimension 0 and 2
```

- struct Center_level_set This is a struct that is only used internally.
- struct Adcection_diffusion_eqn Refer to Section 2.1 for usage of member variables and functions.
- class Population_density The class containing the population density distribution, as a linear combination of particles it contained.
 - Member variables:

where the particle_vector is defined as follows:

```
typedef tbb::concurrent_vector<Particle> particle_vector;
```

Note that p_vect shall be treated as unavailable to access directly out side of the class scope, since the only reason for it to be not private is due to constraints of the tbb library used.

- Constructor

An empty Population_density can be initialized by the following constructor

 Container-related methods: Population_density can be accessed and modified like a vector, with operater [], begin(), end(), size() resize() and iterators as standard vectors.

To add particles to the population, use append to push back particle into the population:

```
particle_vector::iterator append(const Particle& particle) {
    p_vect.push_back(particle);
    //p_vect.insert(end(), particle);
    return end();
}
```

- Evaluation methods

Information about the population can be obtained by using the following functions:

```
value_type density_at (const State_variable& location) const;//returns ↔
population density at location
value_type density_projection_at_coordinate(const State_variable& location ↔
, const std::vector<bool>& range_dimensions) const;//range_dimensions ↔
is of length dimension. e.g. TFTF means projection to dimension 0 and ↔
2
std::vector<value_type> density_at(const std::vector<State_variable>& ↔
location) const;//returns population density at all points in the ↔
location vector
std::vector<value_type> density_projection_at_coordinate(const std::vector ↔
<State_variable>& location, const std::vector<bool>& range_dimensions) ↔
const;//range_dimensions is of length dimension. e.g. TFTF means ↔
projection to dimension 0 and 2
double average_in_index(const int coord_idx) const;//returns the average ↔
value for coordinate i. (e.g. in HH model, average_in_index(0) returns ↔
average membrane potential.
```

- Visualization methods

If the macro MATLAB_VISUALIZE is enabled, then the following plot functions that uses matlab engine is available:

```
Plot_handle plot_density(std::vector<bool> projection_dimensions, const ← value_type x_lb, const value_type x_ub, const value_type y_lb, const ← value_type y_ub, const char* imagesc_options = "") const;

//Plot the marginal population density projected into the ← projection_dimensions.

//e.g.: in a 4-dimensional space, projection_dimensions=TFTF projects the ← marginal density into 1st and 3rd dimension.
```

```
//The projection can be into a 1-dimensional or 2-dimensional subspace
 //x_lb, x_ub, y_lb, y_ub is the lower and bounds for the coordinates to \leftrightarrow
              project to. y_lb, y_ub is not used when projection is into a 1-\leftrightarrow
               dimensional subspace
//imagesc_options passes additional parameters into the imagesc command of ↔
Plot_handle plot_density(const value_type x_lb, const value_type x_ub, ↔
              const value_type y_lb, const value_type y_ub, const char* ← imagesc_options = "") const;
 //project into first 2 dimensions
{\tt Plot\_handle\ plot\_density(const\ int\ projection\_dimension\ ,\ const\ value\_type\ } \hookleftarrow
              \verb|x_lb|, const| value_type x_ub|, const| char *imagesc_options|) const; // \leftarrow | const| char *imagesc_options| char *
               project into 1 dimension
//Plot Flags: 1 overwrite, 2 not plot second eigenvec, 4 not plot first ↔
              eigenvec.
\label{eq:plot_handle} \begin{array}{lll} \texttt{Plot\_handle plot(std::vector} < \texttt{bool} > \texttt{projection\_dimensions} \;,\;\; & \texttt{const} \;\; & \texttt{char*} \;\; & \leftarrow \\ & \texttt{plot\_options} \;=\; "\; , \;\; & \texttt{const} \;\; & \texttt{int} \;\; & \texttt{plot\_flags} \;=\; 1) \;; \\ \texttt{Plot\_handle plot(const} \;\; & \texttt{char*} \;\; & \texttt{plot\_options} \;\; & =\; "\; , \;\; & \texttt{const} \;\; & \texttt{int} \;\; & \texttt{plot\_flags} \;=\; 1) \;; \\ \leftarrow \end{array}
               //project into first 2 dimensions.
{\tt Plot\_handle\ output\_center\_and\_weight()\ const;}
{\tt Plot\_handle\ copy\_particle\_to\_matlab(const\ index\_type\ i)\ const;//COPY} \leftarrow
               single particle to matlab workspace
void output_particle(const index_type i, const char output_filename[] = "← particle.mat") const;//OUTPUT single particle to a mat file
```

- Data I/O methods:

Independent of whether macro MATLAB_VISUALIZE is enabled or not, the following functions allows input and output of population density as linear combination of particles. Please refer to the end of section 2.1 for the format of the files.

```
void output_all_particles(const char output_filename[] = "particles.mat") ←
    const;//OUTPUT particles to a mat or h5 file
void input_all_particles(const char input_filename[] = "particles.mat");//←
INPUT particles to a mat or h5 file
```

- class Population_density_with_equation : public Population_density The class containing a population density, and an advection-diffusion equation, which is an inherited class from Population_density.
 - Additional member variables:

```
const value_type tau;
//tau NOW only affect particle combination. Larger tau leads to less ←
    aggressive particle combination.
const value_type lambda;//regulariztion factor
const value_type alpha;//advection velocity relative distance. alpha small←
    uses level set closer to center.
```

- Constructor:

```
\label{eq:population_density_with_equation} Population_density_with_equation(const Advection_diffusion_eqn\& \leftarrow adv_diff_eqn , const index_type state_space_dimension , const value_type <math display="block"> \begin{array}{c} tau = 0.01 \ / \ 4.0 \ / \ log(2.0) \ , const \ value_type \ lambda = 1e-6, \ const \leftarrow value_type \ alpha = 0.2) \\ \vdots \ Population_density(state_space_dimension) \ , adv_diff_eqn(adv_diff_eqn) \leftarrow \ , \ tau(tau) \ , \ lambda(lambda) \ , \ alpha(alpha) \ \{ \ set_ODE(adv_diff_eqn) \ ; \\ \} \end{array}
```

- Methods for updating population density for timestep:

```
void update_ODE_const (const value_type timestep, const index_type ←
stepcount = 1);//Updates population density with fixed timestep
void update_ODE_adaptive(const value_type timestep, const index_type ←
stepcount = 1);//Update population density with variable timestep that←
is at most timestep
void update_ODE_adaptive_split(const value_type coupling_timestep, const ←
index_type stepcount, const value_type rel_error_bound);//Update ←
population density with variable timestep that is at most timestep. ←
Moreover, if particles are too large to be accurate, particles are ←
splitted automatically
```

- Functions to split and combine particles:

```
void split_particles(const value_type rel_error_bound = ←
    DEFAULT_SPLIT_REL_ERROR);//Split all particles that are too large. No ←
    need to call if using update_ODE_adaptive_split
    void combine_particles();//combine particles. Should be called between ←
    each update_ODE step
```

- Additional helper functions:

```
\begin{array}{lll} \textbf{void} & \textbf{check\_linear\_approx} \big( \textbf{const} & \textbf{int} & \textbf{particle\_index} \big) & \textbf{const}; // \textbf{prints} & \textbf{information} & \hookleftarrow \\ & \textbf{about} & \textbf{accuracy} & \textbf{of} & \textbf{local} & \textbf{linear} & \textbf{approximation} \end{array}
```