OOPS Documentation

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1 Introduction

Let's talk about how scientific codes get written. Some graduate student named Steve has a tough problem to solve, so he learns just enough coding and numerical methods to solve his one problem. The code isn't pretty, but it doesn't have to be because it's simple and easy-to-use for Steve's one problem. Steve eventually graduates, but his advisor, Dr. Fred Smith, holds onto a copy of the code because it works so well.

Now enters Bob, a bright-eyed graduate student with enough stupidity ambition to pursue Dr. Smith's next tough problem and absolutely no coding experience. This tough problem happens to be somewhat similar to Steve's problem, so Dr. Smith starts Bob on Steve's old code. Roughly three months later, Bob has cannibalized Steve's code and extended it to work with his problem, too. It's ugly and gross in every way, but it still runs decently quickly and is simple enough that no one cares. He graduates and quickly forgets about the code.

Dr. Smith repeats this cycle with three or four more graduate students, plus about a dozen undergraduates who pop into his research group along the way. Halfway through, Annie the undergrad notices that the code is an absolute trainwreck and decides to rewrite portions of it. Unfortunately, she has to graduate, so she only rewrites the portions that she needs for her project, and now the code is a horrible amalgam of modern object-oriented programming, Steve's hard-coded relics, and everyone else's half-baked tweaks which never should have seen the light of day. Naturally, the documentation is more sparse

than an SPS activity without free food, so Dr. Smith's students spend half their time trying to decipher what has become known as "The Frankencode."

The Object-Oriented PDE Solver, or OOPS, is designed to alleviate as many of these problems as possible. By creating a flexible object-oriented design, even those relatively inexperienced with coding and numerical methods can quickly solve their problems without ever having to worry about much more than the PDE itself. At the same time, the framework is flexible enough that those who do need to worry about it can.

2 Getting Started with OOPS

Because the OOPS framework is currently so small and lightweight, the entire framework is compiled with each project without any extra library dependencies. We warn the user that this will likely change in a future release as the project grows in scope.

2.1 System Requirements

OOPS requires CMake 3.0 or later and a C++ compiler supporting C++11 or later. Some optional features require the bbhutil library from RNPL. This package is quite old and is only known to work on select Linux distributions (Ubuntu 16.04 and RHEL 7.0 have been tested) after a very onerous installation procedure. We recommend a Linux environment (native, virtual machines, or the Windows Subsystem for Linux should work), but any appropriately configured Windows or MacOS environment should work as well, albeit without the optional features depending on bbhutil.

The procedure for building OOPS in Linux is as follows:

```
cd <path to OOPS base directory>
mkdir build
cd build
ccmake ../
```

A configuration menu should appear. Press ${\tt c}$ to generate the configuration file. The default options should be sufficient. Press ${\tt c}$ again, then ${\tt g}$ to generate the make files.

make

After this, all generated executables should appear in the build directory.

2.2 Structure of OOPS

The most basic OOPS program contains the following components:

- A Domain object, which defines the space for your problem.
- One or more Grid objects, which subdivide a Domain into discrete points for numerical calculation.
- A Solver object, such as RK4, which will numerically solve any PDE fed into it.
- An ODE object, which provides the righthand side for a system of ODEs (such as a PDE discretized with finite-difference methods), boundary conditions, and initial conditions.

More complex codes will also make use of Parameter objects and Interpolator objects, but these are not much more difficult to add in. OOPS works as hard as possible to hide as many of the gory details behind the scenes.

2.3 Solving a Simple Initial Boundary Value Problem

For this project, we'll create a simple program using OOPS that solves the wave equation on a domain with outflow boundaries. Begin by building a new project directory for the program:

cd <path to OOPS base directory>
mkdir WaveEquation
cd WaveEquation
mkdir include
mkdir src

The include folder will contain any header files specific to the WaveEquation program, and src will hold the main file and any additional source files required.

Before we start writing our code, remember that the wave equation in one dimension takes the form

$$\partial_{tt}\phi - \partial_{xx}\phi = 0. (1)$$

OOPS can't solve this in its current form because the time integrator expects it to be first order in space. Therefore, we make the definition $\pi = \partial_t \phi$, which suggests the ODE system

$$\partial_t \phi = \pi, \tag{2}$$

$$\partial_t \pi = \partial_{xx} \phi. \tag{3}$$

OOPS can actually solve this as is because we can just define a second-order derivative operator, but it's just as easy to reduce the spatial order by defining $\chi = \partial_x \phi$, giving us the system

$$\begin{aligned}
\partial_t \phi &= \pi, \\
\partial_t \pi &= \partial_x \chi, \\
\partial_t \chi &= \partial_x \pi,
\end{aligned} \tag{4}$$

where the third equation comes from the commutability of partial derivatives. Despite the two systems being mathematically identical and producing solutions to the wave equation, they exhibit very different numerical properties, with the first-order system being more dispersive and the second-order system being more diffusive.

2.3.1 wave.h

The next step is to construct our PDE. In the include directory, create a new file wave.h that reads as follows:

```
#ifndef WAVE_H
           #define WAVE_H
2
           #include <ode.h>
           class Wave : public ODE {
             private:
               // Variable labels
               static const unsigned int U_PHI = 0;
               static const unsigned int U_PI = 1;
               static const unsigned int U_CHI = 2;
11
12
13
             protected:
               virtual void applyBoundaries(bool intermediate);
14
               virtual void rhs(const Grid& grid, double **u, double←
16
                     **dudt);
17
             public:
18
               Wave(Domain& d, Solver& s);
               virtual ~Wave();
20
21
               virtual void initData();
22
           };
23
24
           #endif
```

The ode.h file defines the ODE object, which defines an abstract class representing a system of ODEs (or a discretized system of PDEs). We declare a new class, Wave, which inherits from ODE and therefore reduces a lot of the work that we have to do.

Underneath the **private** label, we assign some variable names to our specific indices. This isn't necessary, strictly speaking, but it makes your code a lot more readable when we start writing the righthand-side routine.

For our protected methods, we have two virtual functions, applyBoundaries() and rhs(), which are both inherited from ODE. The method applyBoundaries() is used in the evolution function (which is also virtual and can be overwritten, but the default definition works well enough for this case) to fix the boundaries between each stage of the Solver object we'll attach later. The intermediate flag will be explained in more detail later, but it has to do with figuring out

which data set needs to be modified. The rhs() method contains the righthand side of Eq. (4).

Lastly, inside the public region, we have a constructor and a destructor as well as initData(), which contains the initial data for the ODE. This is made public for convenience, as more advanced implementations may have a custom Parameter object, which can be used, among other things, to control the initial conditions for a specific ODE.

2.3.2 wave.cpp

The next file we need to create is wave.cpp, which is located inside src and contains the definitions for wave.h. We'll take this one piece at a time:

```
#include <wave.h>
#include <operators.h>
#include <iostream>
#include <cmath>
```

Clearly wave.h is the header file we just created. The file operators.h contains a set of pre-defined derivative operators. Next, we need access to the I/O and math functions from the Standard Template Library, so we go ahead and include those.

```
// Constructor
           Wave:: Wave (Domain& d, Solver& s) : ODE (3, 0) {
3
             if(d.getGhostPoints() < 2)
               std::cerr << "Warning: domain has fewer ghost points ←
                   than expected. Expect incorrect behavior.\n";
6
             domain = \&d;
             solver = \&s;
             // Set some default parameters.
10
             params = new Parameters();
11
12
             reallocateData();
13
14
15
           // Destructor
16
17
           Wave::\simWave(){
             delete params;
18
```

When we define our constructor, we have to make sure that we call the ODE constructor, ODE(const unsigned int n, const unsigned int id). The first argument, n, is the number of variables for our ODE object, and id is an identifier. For our simple program, id isn't really important, but it's a sort of baroque method for manually type-checking Parameters types and ODE objects. Basically id=0 just means that we can use the default Parameters object.

We are going to construct our ODE method with fourth-order derivative operators, so we need at least two ghost points at the boundaries to ensure that we get fourth-order accuracy. The if statement guarantees that this is the case and spits out an error promising that the solution will behave incorrectly.

Next, we need to set the domain and solver for our ODE. This should always be done in the constructor so that memory is allocated properly.

We then build a Parameters object for our ODE. The default Parameters object is very simple and basically just stores information about what sort of Interpolator should be used, (which is not important for our particularly simple example), but a custom Parameters object could also contain information about what order derivative operators to use, initial conditions, and so forth.

The last line needs a little bit of explanation. Whenever we assign a Domain object to our ODE, we need to allocate memory for every single variable at every single point. If this is done for a multi-stage Solver, such as RK4, we also need to allocate this same amount of memory for each stage. Therefore, any time the Domain or Solver objects are changed, ODE automatically calls reallocateData(). When an ODE object is destroyed, it automatically deallocates this memory. However, the constructor doesn't automatically call this routine because we assign the Domain and Solver manually rather than through the setDomain() and setSolver() methods, therefore we must explicitly call reallocateData().

The destructor doesn't need to do much because most of the heavy lifting is handled by ODE. Therefore, the only thing we need to do is call delete on the Parameters object we created.

The next piece we need to implement is the rhs() function:

```
void Wave::rhs(const Grid& grid, double **u, double **←
                 dudt){
               // Go ahead and define some stuff we will need.
               double stencil3[3] = \{0.0, 0.0, 0.0\};
               double stencil5[5] = \{0.0, 0.0, 0.0, 0.0, 0.0\};
               double dx = grid.getSpacing();
               int shp = grid.getSize();
               // Calculate the left boundary. We switch to a \hookleftarrow
                    different operator on the boundaries, which should
               // just be ghost points that will be overwritten, \leftarrow
                    anyway.
               // Leftmost point.
10
               {\tt dudt} \, [\, {\tt U\_PHI} \, ] \, [\, 0\, ] \,\, = \, {\tt u} \, [\, {\tt U\_PI} \, ] \, [\, 0\, ] \, ;
11
                            = u[U_CHI][0];
               stencil3[0]
12
               stencil3[1] = u[U_CHI][1];
13
               stencil3[2] = u[U_CHI][2];
14
               dudt[U_PI][0] = operators::dx_2off(stencil3, dx);
15
               stencil3[0] = u[U_PI][0];
stencil3[1] = u[U_PI][1];
16
17
               stencil3[2] = u[U_PI][2];
18
               dudt[U_CHI][0] = operators::dx_2off(stencil3, dx);
19
20
               // Second leftmost point.
21
```

```
dudt[U_PHI][1] = u[U_PI][1];
22
                   stencil3[0] = u[U_CHI][0];
23
                   stencil3[1] = u[U_CHI][1];
24
                   stencil3[2] = u[U_CHI][2];
25
                   dudt[U_PI][1] = operators::dx_2(stencil3, dx);
26
                   stencil3[0] = u[U_PI][0];
stencil3[1] = u[U_PI][1];
27
28
                   stencil3\begin{bmatrix} 2 \end{bmatrix} = u \begin{bmatrix} U_PI \end{bmatrix} \begin{bmatrix} 2 \end{bmatrix};
29
                   dudt[U_CHI][1] = operators::dx_2(stencil3, dx);
30
31
                    // Now set all the interior points.
32
                    for (int i = 2; i < shp - 2; i++){
33
                       dudt[U_PHI][i] = u[U_PI][i];
34
                       for(int j = 0; j < 5; j++){
36
                          stencil5[j] = u[U_CHI][i - 2 + j];
37
38
                      dudt[U_PI][i] = operators::dx_4(stencil5, dx);
39
                       for(int j = 0; j < 5; j++){}
41
                          stencil5[j] = u[U_PI][i - 2 + j];
42
43
                       \mathtt{dudt} \, [\, \mathtt{U\_CHI} \, ] \, [\, \mathtt{i} \, ] \, = \, \mathtt{operators} :: \mathtt{dx\_4} \, (\, \mathtt{stencil5} \, \, , \, \, \mathtt{dx} \, ) \, ;
44
                   }
45
46
                    // Second rightmost point.
47
                   dudt[U_PHI][shp - 2] = u[U_PI][shp - 2];
48
                   stencil3[0] = u[U_CHI][shp - 3];
49
50
                   stencil3[1] = u[U_CHI][shp - 2];
                   stencil3[2] = u[U_CHI][shp - 1];
51
                   dudt[U_PI][shp - 2] = operators :: dx_2(stencil3, dx);
52
                   stencil3 [0] = u[U_PI][shp - 3];
53
                   stencil3[1] = u[U_PI][shp - 2];
54
55
                   stencil3[2] = u[U_PI][shp - 1];
                   dudt[U_CHI][shp - 2] = operators::dx_2(stencil3, dx);
56
57
                    // Rightmost point.
58
                   dudt[U_PHI][shp - 1] = u[U_PI][shp - 1];
59
                   \mathtt{stencil3} \hspace{.05cm} [\hspace{.05cm} 0 \hspace{.05cm}] \hspace{.1cm} = \hspace{.1cm} \mathtt{u} \hspace{.05cm} [\hspace{.05cm} \mathtt{U\_CHI} \hspace{.05cm}] \hspace{.05cm} [\hspace{.05cm} \mathtt{shp} \hspace{.1cm} - \hspace{.1cm} 3 \hspace{.05cm}] \hspace{.05cm} ;
60
                   stencil3[1] = u[U_CHI][shp - 2];
stencil3[2] = u[U_CHI][shp - 1];
61
62
                   dudt[U_PI][shp - 1] = operators :: dx_2off(stencil3, dx);
63
                   \mathtt{stencil3} \, [\, \dot{0} \, ] \, = \, \mathtt{u} \, [\, \mathtt{U\_PI} \, ] \, [\, \mathtt{shp} \, - \, 3 \, ] \, ;
                   {\tt stencil3}\,[\,1\,] \;=\; {\tt u}\,[\,{\tt U\_PI}\,]\,[\,{\tt shp}\ -\ 2\,]\,;
65
                                     = u[U_PI][shp - 1];
66
                    stencil3[2]
                   dudt[U_CHI][shp - 1] = operators::dx_2off(stencil3, dx);
67
68
```

This piece of code is somewhat long, but it's quite straightforward. Basically, we manually set the left and right boundaries using second-order derivative operators, which require a 3-point stencil, and all the interior points use a full fourth-order operator with a 5-point stencil. Every derivative operator takes an appropriately sized stencil and spatial interval.

After setting up the righthand side, we still need to define some boundary conditions. We're assuming a Neumann boundary, so this is easy to set up.

```
void Wave::applyBoundaries(bool intermediate){
              unsigned int nb = domain->getGhostPoints();
2
              // Grab the data at the leftmost grid and the rightmost ←
3
                    grid.
              auto left_it = data.begin();
              auto right_it = --data.end();
6
              double **left;
              double **right;
              if (!intermediate) {
10
                left = left_it->getData();
11
                right = right_it->getData();
12
13
              else{
                left = left_it->getIntermediateData();
15
                right = right_it->getIntermediateData();
16
17
              unsigned int nr = right_it->getGrid().getSize();
18
19
              // Apply Neumann boundary condition.
20
              for (unsigned int i = 0; i < nb; i++){
21
                \label{eq:left_u_PHI} \texttt{left[U_PHI][i]} \, = \, \texttt{left[U_PHI][nb]};
22
                left[U_PI][i] = left[U_PI][nb];
23
24
                left[U_CHI][i] = 0.0;
25
26
                right [U_PHI][nr - 1 - i] = right [U_PHI][nr - 1 - i];
                right[U_PI][nr - 1 - i] = right[U_PI][nr - 1 - i];
27
                right[U_CHI][nr - 1 - i] = 0;
28
              }
29
            }
30
```

This is a great time to explain how spatial data is stored in OOPS. Every Domain contains one or more Grid objects, which are stored in a std::treeset and sorted from left to right. Every ODE object maintains a set of SolverData objects, each of which are assigned a specific grid, and are also sorted from left to right. This makes it possible to store multiple grids on a single domain, thus allowing for different-sized grids in different regions of the solution. Hypothetically, this allows for adaptive mesh refinement, although that feature has not been implemented yet.

In any case, we need to make sure that we retrieve the leftmost and rightmost grids on the domain, because those will be the ones containing the physical boundaries. If we're using a multi-stage Solver object, the intermediate flag tells us whether this data needs to come from the intermediate data stored between stages or the original data from the beginning of the time step. After that, applying the boundary condition itself is nearly trivial. Because we have a Neumann boundary, we set $\chi = \partial_x \phi = 0$, and we enforce this same condition in ϕ and π by copying the physical boundary into the ghost points.

The last piece for this file is setting the initial conditions. For simplicity, we'll assume a Gaussian centered around x = 0.5. The code looks like this:

```
void Wave::initData(){
1
               // The center of our Gaussian.
               double x0 = 0.5:
3
               // Loop through every grid and start assigning points.
               for(auto it = data.begin(); it != data.end(); ++it){
6
                 const double *x = it->getGrid().getPoints();
                 unsigned int nx = it->getGrid().getSize();
                 double **u = it->getData();
10
                 for (unsigned int i = 0; i < nx; i++){
                   double val = std::exp(-(x[i] - x0)*(x[i] - x0)*64.0);
11
                   u[U_PHI][i] = val;
12
                   u[U_PI][i] = 0.0;
13
                   {\tt u\,[\,U\_CHI\,]\,[\,i\,]} \ = \ -1\,2\,8\,.\,0\,*\,(\,{\tt x\,[\,i\,]} \ -\ {\tt x\,0}\,)\,*\,{\tt v\,al}\,;
15
              }
16
17
            }
```

After our discussion on boundary conditions, the purpose of the loop should be more straightforward: we need to loop over every grid on our domain so we can set each of their points fit along a Gaussian.

2.3.3 main.cpp

We're in the home stretch! With our ODE set up, all that's left is our main() function. Start by making a new file in the src directory called main.cpp.

```
#include <domain.h>
            #include <grid.h>
2
3
            #include <rk4.h>
            #include <cmath>
4
            #include <cstdio>
            #include <wave.h>
            \#include <polynomialinterpolator.h>
            int main(int argc, char* argv[]){
9
               // Construct our domain and a grid to fit on it.
10
11
               Domain domain = Domain();
               int N = 101;
12
               {\tt domain.addGrid} \, (\, {\tt domain.getBounds} \, (\, ) \,\, , \,\, \, {\tt N} \, ) \,\, ;
13
14
               // Set up our ODE system.
15
               RK4 rk4 = RK4();
16
               PolynomialInterpolator interpolator = \leftarrow
17
                    PolynomialInterpolator (4);
               Wave ode = Wave(domain, rk4);
18
               ode.setInterpolator(&interpolator);
19
               ode.initData();
20
21
               double ti = 0.0;
22
               double tf = 5.0;
23
               \texttt{doublt} \ \texttt{dt} = \texttt{domain.getCFL}()*(--\texttt{domain.getGrids}().\texttt{end}()) -> \leftarrow
                    getSpacing();
               unsigned int M = (tf - ti)/dt;
25
               ode.dump_csv("phi00000.csv", 0, 0);
```

```
for (unsigned int i = 0; i < M; i++){
27
                double t = (i + 1)*dt;
28
                ode.evolveStep(dt);
29
30
                char buffer [12];
31
                sprintf(buffer, "phi%05d.csv",i+1);
32
33
                ode.dump_csv(buffer, t, 0);
34
              return 0;
36
37
```

Inside the main function, we can see the procedure for constructing a Domain. When we create a new Domain object, it is generated with some defaults. The boundaries are automatically defined at x=0 and x=1.0, the number of ghost points is set to 3, and we have a Courant-Friedrichs-Lewy (CFL) factor of 0.5. This helps us set the time step to something guaranteed to be stable for our chosen spatial interval, although in practice this depends a lot on the particular equation we're solving. We can add a Grid to the Domain with the method addGrid(double bounds[2], unsigned int n), where bounds defines the spatial location of the Grid (which, in this case, is just the entire domain) and the number of physical points for the Grid. Now is a good time to note that the number of actual points on the grid is going to be n + 2*nghosts, where nghosts is the number of ghost points, which will extend slightly beyond the region specified by bounds[].

The next step is constructing our Wave ODE object. We first start by picking a Solver for the time integration, which is RK4 in this case. We then construct an Interpolator object because it's required by the ODE class to transfer data between different-sized Grid objects, although this functionality is not important for our purposes. We then build our Wave object, assign the new Interpolator, and set the initial data.

Finally, we need to run our main loop. We calculate our time step, the number of total steps (because calculating t from the number of steps is less prone to numerical error than adding dt over and over), and run evolveStep(dt). We also dump our data to a .csv file every step so we can look at the results when we're done.

2.3.4 Compiling the Project

By the end of this, you're asking, "We're done, right?"

The answer to that question is yes and no. We're done writing C++, but we still have one more step before we can compile our code and run the project. So, navigate to the OOPS base directory and open up CMakeLists.txt. Append the following to the end of the file:

```
set(WAVE_INCLUDE_FILES
Wave/include/wave.h
)
```

```
set (TEST_SOURCE_FILES
4
                Wave/src/wave.cpp
               Wave/src/main.cpp
6
           set(SOURCE_FILES \${GRID_SOURCE_FILES} \${ ↔
               GRID_INCLUDE_FILES \${TEST_SOURCE_FILES} \${\Leftrightarrow}
               WAVE_INCLUDE_FILES })
           add_executable(Wave \${SOURCE_FILES})
11
           target_link_libraries(Wave \${EXTRA_LIBS})
           target_include_directories(Wave PUBLIC \
12
               CMAKE_CURRENT_SOURCE_DIR \} / include
                                         \${CMAKE_CURRENT_SOURCE_DIR}/
13
                                             Wave/include \ \longleftrightarrow
                                             PROJECT_SOURCE_DIR })
```

After that, rerun CMake, compile, and you should have an executable, Wave, which will solve your wave equation when you run it.

2.3.5 Afterthoughts

By this time, you're saying, "You said this would be simple! Why did it take so long? This seems like overkill for such a simple problem."

You're probably right. If all you're trying to do is solve the wave equation, you really don't need all this machinery. But let's start by talking about all the things you didn't have to do. You didn't have to write your own numerical integrator, first of all. You just loaded up the standard RK4 integrator, attached it to the Wave object, and you were good to go. You also didn't have to worry about discretizing the Domain yourself. This isn't a terribly difficult process if all you need is a single uniform grid, but it takes out one more failing point in your code. You didn't have to write your own derivative operators. Again, these aren't difficult, but they do take time, especially if you want something more than the traditional second-order centered finite-difference operators. You didn't have to worry about boundary conditions getting applied correctly between the different stages of the numerical integrator, either; you just overloaded applyBoundaries, wrote out the boundaries you wanted, and let OOPS do the rest for you.

Now let's talk about what you can do thanks to OOPS. By just changing a few lines of code in your main function, you could change your problem from a single grid to three or four grids, perhaps to give you good resolution in the middle where the peak of the Gaussian is located and less resolution toward the edges where the data is more flat. OOPS automatically handles the data transfer between neighboring grids, including interpolating between different-sized grids (so long as they're a multiple of two apart). If the RK4 integrator isn't good enough for your problem, you can write a new integrator using the Solver base class with just three functions (two of which are nearly identical). It will automatically work with all the rest of the OOPS machinery. If you're working on a complicated problem that requires some extra steps in the evolution method (ODE::evolveStep()), you can do that with the doAfter...() methods.

3 Documentation

3.1 Domain Class

The Domain class defines the physical region a PDE should be solved on. It acts as a factory for Grid objects and contains the necessary parameters to construct them appropriately.

Public Methods

- Domain() The constructor for a Domain object. By default, it sets the number of ghost points to three, the boundaries to [0,1], and the CFL factor to 0.5.
- ~Domain() The destructor for a Domain object. It automatically clears all grids attached to the Domain.
- void setCFL(double cf1) Set the CFL factor. At the moment, this doesn't affect anything in the code itself. Future releases may use this to calculate a recommended time step.
- double getCFL() const Get the CFL factor.
- void setBounds(double bounds[2]) Set the bounds for the domain with an ordered pair. This will also clear any Grid objects still on the Domain.
- const double* getBounds() const Get the bounds for the Domain as an ordered pair.
- void setGhostPoints(unsigned int n) Set the number of ghost points to use while constructing new Grid objects. This will clear any Grid objects still on the Domain.
- unsigned int getGhostPoints() const Get the number of ghost points used while constructing new Grid objects.
- std::set<Grid>& getGrids() Get a set containing all the different Grid
 objects currently on the Domain.
- Result addGrid(double bounds[2], unsigned int n) Using an ordered pair bounds[], add a new Grid with n uniformly spaced points to the Domain. It returns SUCCESS if it succeeded and BAD_ALLOC if it failed.
- void clearGrids() Clear all Grid objects currently on the Domain.

3.2 Grid Class

The Grid class defines a 1d grid with uniform spacing. These are the building blocks for basically all calculations in OOPS.

Public Methods

- Grid(const double bounds[2], unsigned int n, unsigned int nghosts)

 The constructor for a new Grid with n points from bounds[0] to bounds[1],
 plus an additional nghosts ghost points on either end.
- Grid(const Grid& other) The copy construct for Grid. Because memory is allocated and deallocated in every Grid object, this performs a deep copy.
- ~Grid() This is the destructor for the Grid class. It frees all the memory allocated for the Grid points.
- Result rebuildGrid(const double bounds[2], unsigned int n, unsigned int nghosts) A function to rebuild a Grid, with the arguments being the same as the constructor, if something needs to change. It returns SUCCESS on success and BAD_ALLOC if it fails.
- const double* getPoints() const Get the array containing the physical location of every grid point.
- const unsigned int getSize() const Get the number of points, including ghost points, currently on the grid.
- const double getSpacing() const Get the space interval between points.
- const double* getBounds() const Get the bounds, excluding ghost points,
 of the Grid as an ordered pair.
- bool operator < (const Grid& g) const Compare two Grid objects to each other. If the right bound for the Grid on the left side of the operator is less than the left bound for the Grid on the right side of the operator, this returns true. If the two Grid objects overlap at all, this will always return false, even if you flip the arguments.
- Boundary whichNeighbor(const Grid& g) const If two Grid objects share a boundary, this will return Boundary::LEFT or Boundary::RIGHT. Otherwise, it returns Boundary::NONE.

3.3 Solver Class

The Solver class is an interface for numerical integrators. As such, it cannot be instantiated, but any numerical integrator, such as the included RK4 integrator, must be a descendant of the Solver class to work properly with the rest of the OOPS machinery. This particular class may be rewritten somewhat in the future to make it more consistent with the rest of OOPS.

Protected Fields

const int nStages The number of stages for the Solver, which is specified in the constructor.

Public Methods

Solver(const int n) A basic constructor included to set the number of stages for a Solver. All subclasses must call this constructor in their initialization list.

int getNStages() const Get the number of stages for the Solver.

Unimplemented Public Methods

virtual Result calcStage(void (*rhs)(const Grid&, double**, double**), double *data0[], double *dataint[], double *dest[], const Grid& grid, double dt, const unsigned int vars, unsigned int stage)

This method must be implemented for compability with older procedural tests, but it is deprecated and will be removed in a future release. The first argument is a function pointer to a righthand-side function. The data0[] argument is a 2d array which includes the original data from the beginning of the time step. The dataint[] argument is also a 2d array, but it stores intermediate data from the previous stage in the integrator. The dest[] argument is also a 2d array where the result from the stage is stored. You also specify a Grid to pass into the righthand-side function, a timestep dt, the number of variables for the righthand-side, and the current stage of the solver.

virtual Result calcStage(ODE *ode, double *data0[], double *dataint[], double *dest[], const Grid& grid, double dt, unsigned int stage)

This is the method currently used by the OOPS framework for calculating each stage of a Solver object. The arguments are very similar to the function above, but the function pointer is replaced by a pointer to an ODE, which contains the righthand-side function and the number of variables (which is also missing). Because this function is used inside a loop over the different Grid objects, the data and Grid must still be included explicitly, but a future release may modify this to move the loop into the Solver itself.

virtual Result combineStages(double **data[], double *dest[], const
 Grid& grid, double dt, const int vars) This function combines all
 the stages together. The data[] array is organized by [STAGE][VAR][INDEX]
 and contains all the work data from the previous calculations. The dest[]
 array contains the final result of the calculation. The Grid for this calculation is supplied, as is the time step and the number of variables for the
 equation.

3.4 ODE Class

ODE is an abstract class describing a generic system of differential equations. As a brief note, no ODE object is copyable because they store a considerable amount of dynamically allocated memory.

Protected Fields

- const unsigned int nEqs The number of independent equations in this system.
- const unsigned int pID The ID associated with this ODE. This is used for identifying compatible Parameter objects.
- Parameters *params A pointer to the Parameter object associated with the ODE
- Domain *domain The Domain this ODE is being solved on. This is how the ODE accesses all of the Grid objects it needs to construct the SolverData objects.
- std::set<SolverData> data A set containing all the SolverData objects for
 each Grid.
- Solver *solver The Solver that should be used to calculate each step.
- Interpolator *interpolator The Interpolator used to transfer solution data between differently sized Grid objects.
- max_dx The maximum grid spacing across all Grid objects on the Domain.

Protected Methods

- virtual void applyBoundaries(bool intermediate) A function to apply boundary conditions after data is transferred between Grid objects. It is empty by default, so initial value problems don't need to implement this at all.
- virtual void doAfterStage(bool intermediate) An empty function which can be overwritten to perform specific tasks after the Solver stage completes but before the Grid exchange occurs.
- virtual void doAfterExchange(bool intermediate) An empty function which can be overwritten to perform specific tasks after the Grid exchange occurs but before the boundaries are applied.
- virtual void doAfterBoundaries(bool intermediate) An empty function which can be overwritten to perform specific tasks after the boundary conditions are applied but before the next stage is calculated.
- Result reallocateData() A function that clears and reallocates all of the data. This may be important if the Domain or any of its Grid objects change.
- void performGridExchange() This exchanges data between the ghost points
 of neighboring Grid objects, including taking care of interpolation.

- void interpolateLeft(const SolverData &datal, const SolverData &datar) A helper function for interpolation that assumes the SolverData to the left of the interface is finer.
- void interpolateRight(const SolverData &datal, const SolverData &datar)
 A helper function for interpolation that assumes the SolverData to the right of the interface is finer.

Public Methods

- ODE(const unsigned int n, const unsigned int id) The constructor for ODE, which all subclasses must call in their initialization lists, which defines a new ODE object with n equations utilizing Parameter objects with the provided id.
- ~ODE() The destructor for the ODE, which clears all the data.
- Result setDomain(Domain *domain) Set the Domain for the ODE. This will clear all existing data and reallocate it for the new Domain. It returns SUCCESS on success and an error, usually BAD_ALLOC, on failure.
- Result setSolver(Solver *solver) Set the Solver for the ODE. This will clear all existing data and reallocate it for the new Solver. It returns SUCCESS on success and an error, usually BAD_ALLOC, on failure.
- Result setInterpolator(Interpolator *interp) Set the interpolation method used by this ODE. It returns SUCCESS on success and an error on failure, usually BAD_ALLOC.
- virtual Result evolveStep(double dt) The evolution function for a single step. It is overwriteable in case a specific use-case scenario requires more flexibility than the default evolution function provides, but this is not a typical use-case scenario.
- Result setParameters Set the Parameters object for the ODE. If the Parameters object's id matches the ODE's, it returns SUCCESS. Otherwise, it returns UNRECOGNIZED_PARAMS.
- unsigned int getNEqs() const Get the number of equations in the ODE system.
- Domain *getDomain() Get the current Domain used by the ODE.
- Parameters *getParameters Get the current Parameters object used by the ODE.

void output_frame(char *name, double t, unsigned int var) Write out
the data from variable var labeled with time t to <name>.sdf. This
requires the bbhutil library and must be explicitly enabled with the
USE_SDF option during the configuration. Otherwise, a warning is printed
the first time it is called and no data is saved.

dump_csv(char *name, double t, unsigned int var) All the data is dumped to the specified file for the corresponding variable var in the format (t, x, data).

Unimplemented Public Methods

virtual void initData() The initial conditions for the ODE.

virtual void rhs(const Grid& grid, double** data, double** dudt) The righthand-side function for this ODE. It takes a Grid object and the data corresponding to that Grid, then stores the calculated righthand-side in dudt.