
amrex Documentation

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AMReX Team

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AMReX is a software framework library containing all the functionality to write massively parallel, block-structured adaptive mesh refinement (AMR) applications. AMReX is freely available [on Github](#).

AMReX is developed at LBNL, NREL, and ANL as part of the Block-Structured AMR Co-Design Center in DOE's Exascale Computing Project.

All of AMReX's development is done in the github repository under the development branch; anyone can see the latest updates. Changes are merged into the master branch at the beginning of each month.

We are always happy to have users contribute to the AMReX source code. To contribute, issue a pull request against the development branch (details [here](#)). Any level of changes are welcomed: documentation, bug fixes, new test problems, new solvers, etc...

To obtain help, simply post an [issue](#) on the AMReX GitHub webpage.

Besides this documentation, there is API documentation generated by [Doxygen](#).

Documentation on migration from BoxLib is available in the AMReX repository at Docs/Migration.

AMREX INTRODUCTION

AMReX is a publicly available software framework designed for building massively parallel block-structured adaptive mesh refinement (AMR) applications.

Key features of AMReX include:

- C++ and Fortran interfaces
- 1-, 2- and 3-D support
- Support for cell-centered, face-centered, edge-centered, and nodal data
- Support for hyperbolic, parabolic, and elliptic solves on hierarchical adaptive grid structure
- Optional subcycling in time for time-dependent PDEs
- Support for particles
- Support for embedded boundary (cut cell) representations of complex geometries
- Parallelization via flat MPI, OpenMP, hybrid MPI/OpenMP, or MPI/MPI
- Parallel I/O
- Plotfile format supported by AmrVis, VisIt, ParaView, and yt.

AMReX is developed at LBNL, NREL, and ANL as part of the Block-Structured AMR Co-Design Center in DOE's Exascale Computing Project.

GETTING STARTED

In this chapter, we will walk you through two simple examples. It is assumed here that your machine has GNU Make, Python, GCC (including gfortran), and MPI, although AMReX can be built with CMake and other compilers.

2.1 Downloading the Code

The source code of is available at <https://github.com/AMReX-Codes/amrex>. The GitHub repo is our central repo for development. The development branch includes the latest state of the code, and it is merged into the master branch on a monthly basis. The master branch is considered the release branch. The releases are tagged with version number YY.MM (e.g., 17.04). The MM part of the version is incremented every month, and the YY part every year. Bug fix releases are tagged with YY.MM.patch (e.g., 17.04.1).

2.2 Example: Hello World

The source code of this example is at `amrex/Tutorials/Basic>HelloWorld_C/` and is also shown below.

```
#include <AMReX.H>
#include <AMReX_Print.H>

int main(int argc, char* argv[])
{
    amrex::Initialize(argc,argv);
    amrex::Print() << "Hello world from AMReX version "
                  << amrex::Version() << "\n";
    amrex::Finalize();
}
```

The main body of this short example contains three statements. Usually the first and last statements for the `int main(...)` function of every program should be calling `amrex::Initialize` and `amrex::Finalize`, respectively. The second statement calls `amrex::Print` to print out a string that includes the AMReX version returned by the `amrex::Version` function. The example code includes two AMReX header files. Note that the name of all AMReX header files starts with `AMReX_` (or just `AMReX` in the case of `AMReX.H`). All AMReX C++ functions are in the `amrex` namespace.

2.2.1 Building the Code

You build the code in the `amrex/Tutorials/Basic>HelloWorld_C/` directory. Typing `make` will start the compilation process and result in an executable named `main3d.gnu.DEBUG.ex`. The name shows that the GNU compiler with debug options set by AMReX is used. It also shows that the executable is built for 3D. Although this

simple example code is dimension independent, dimensionality does matter for all non-trivial examples. The build process can be adjusted by modifying the `amrex/Tutorials/Basic>HelloWorld_C/GNUmakefile` file. More details on how to build AMReX can be found in [Building AMReX](#).

2.2.2 Running the Code

The example code can be run as follows,

```
./main3d.gnu.DEBUG.ex
```

The result may look like,

```
Hello world from AMReX version 17.05-30-g5775aed933c4-dirty
```

The version string means the current commit 5775aed933c4 (note that the first letter g in g577.. is not part of the hash) is based on 17.05 with 30 additional commits and the AMReX work tree is dirty (i.e. there are uncommitted changes).

In the GNUmakefile there are compilation options for DEBUG mode (less optimized code with more error checking), dimensionality, compiler type, and flags to enable MPI and/or OpenMP parallelism. If there are multiple instances of a parameter, the last instance takes precedence.

2.2.3 Parallelization

Now let's build with MPI by typing `make USE_MPI=TRUE` (alternatively you can set `USE_MPI=TRUE` in the `GNUmakefile`). This should make an executable named `main3d.gnu.DEBUG.MPI.ex`. Note MPI in the file name. You can then run,

```
mpiexec -n 4 ./main3d.gnu.DEBUG.MPI.ex amrex.v=1
```

The result may look like,

```
MPI initialized with 4 MPI processes  
Hello world from AMReX version 17.05-30-g5775aed933c4-dirty
```

If the compilation fails, you are referred to [Building AMReX](#) for more details on how to configure the build system. The *optional* command line argument `amrex.v=1` sets the AMReX verbosity level to 1 to print the number of MPI processes used. More details on how runtime parameters are handled can be found in section [ParmParse](#).

If you want to build with OpenMP, type `make USE_OMP=TRUE`. This should make an executable named `main3d.gnu.DEBUG.OMP.ex`. Note OMP in the file name. Make sure the `OMP_NUM_THREADS` environment variable is set on your system. You can then run,

```
OMP_NUM_THREADS=4 ./main3d.gnu.DEBUG.OMP.ex amrex.v=1
```

The result may look like,

```
OMP initialized with 4 OMP threads  
Hello world from AMReX version 17.06-287-g51875485fe51-dirty
```

Note that you can build with both `USE_MPI=TRUE` and `USE_OMP=TRUE`. You can then run,

```
OMP_NUM_THREADS=4 mpiexec -n 2 ./main3d.gnu.DEBUG.MPI.OMP.ex
```

The result may look like,

```
MPI initialized with 2 MPI processes
OMP initialized with 4 OMP threads
Hello world from AMReX version 17.06-287-g51875485fe51-dirty
```

2.3 Example: Heat Equation Solver

We now look at a more complicated example at `amrex/Tutorials/Basic/HeatEquation_EX1_C` and show how simulation results can be visualized. This example solves the heat equation,

$$\frac{\partial \phi}{\partial t} = \nabla^2 \phi$$

using forward Euler temporal integration on a periodic domain. We could use a 5-point (in 2D) or 7-point (in 3D) stencil, but for demonstration purposes we spatially discretize the PDE by first constructing (negative) fluxes on cell faces, e.g.,

$$F_{i+1/2,j} = \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta x},$$

and then taking the divergence to update the cells,

$$\phi_{i,j}^{n+1} = \phi_{i,j}^n + \frac{\Delta t}{\Delta x} (F_{i+1/2,j} - F_{i-1/2,j}) + \frac{\Delta t}{\Delta y} (F_{i,j+1/2} - F_{i,j-1/2})$$

The implementation details of the code are discussed in section [Example: HeatEquation_EX1_C](#). For now let's just build and run the code, and visualize the results.

2.3.1 Building and Running the Code

To build a 2D executable, go to `amrex/Tutorials/Basic/HeatEquation_EX1_C/Exec` and type `make DIM=2`. This will generate an executable named `main2d.gnu.ex`. To run it, type,

```
./main2d.gnu.ex inputs_2d
```

Note that the command takes a file `inputs_2d`. The calculation solves the heat equation in 2D on a domain with 256×256 cells. It runs 10,000 steps and makes a plotfile every 1,000 steps. When the run finishes, you will have a number of plotfiles, `plt00000`, `plt01000`, etc, in the directory where you are running. You can control runtime parameters such as how many time steps to run and how often to write plotfiles by setting them in `inputs_2d`.

2.4 Visualization

There are several visualization tools that can be used for AMReX plotfiles. One standard tool used within the AMReX-community is Amrvis, a package developed and supported by CCSE that is designed specifically for highly efficient visualization of block-structured hierarchical AMR data. (Amrvis can also be used to visualize performance data; see the [AMReX-based Profiling Tools](#) chapter for further details.) Plotfiles can also be viewed using the VisIt, ParaView, and yt packages. Particle data can be viewed using ParaView. Refer to Chapter on [Visualization](#) for how to use each of these tools.

BUILDING AMREX

In this chapter, we discuss AMReX’s build systems. There are three ways to use AMReX. Most AMReX developers use GNU Make. With this approach, there is no installation step; application codes adopt AMReX’s build system and compile AMReX while compiling their own codes. This will be discussed in more detail in the section on *Building with GNU Make*. The second approach is to build install AMReX as a library (*Building libamrex*); an application code then uses its own build system and links to AMReX as an external library. Finally, AMReX can also be built with CMake, as detailed in the section on *Building with CMake*.

3.1 Building with GNU Make

In this build approach, you write your own make files defining a number of variables and rules. Then you invoke `make` to start the building process. This will result in an executable upon successful completion. The temporary files generated in the building process are stored in a temporary directory named `tmp_build_dir`.

3.1.1 Dissecting a Simple Make File

An example of building with GNU Make can be found in `amrex/Tutorials/Basic/HelloWorld_C`. Table 3.1 below shows a list of important variables.

Table 3.1: Important make variables

| Variable | Value | Default |
|-------------------------|-------------------------------------|-------------|
| <code>AMREX_HOME</code> | Path to amrex | environment |
| <code>COMP</code> | gnu, cray, ibm, intel, llvm, or pgi | none |
| <code>DEBUG</code> | TRUE or FALSE | TRUE |
| <code>DIM</code> | 1 or 2 or 3 | none |
| <code>USE_MPI</code> | TRUE or FALSE | FALSE |
| <code>USE_OMP</code> | TRUE or FALSE | FALSE |

At the beginning of `amrex/Tutorials/Basic/HelloWorld_C/GNUmakefile`, `AMREX_HOME` is set to the path to the top directory of AMReX. Note that in the example `?=` is a conditional variable assignment operator that only has an effect if `AMREX_HOME` has not been defined (including in the environment). One can also set `AMREX_HOME` as an environment variable. For example in bash, one can set

```
export AMREX_HOME=/path/to/amrex
```

alternatively, in tcsh one can set

```
setenv AMREX_HOME /path/to/amrex
```

One must set the `COMP` variable to choose a compiler. Currently the list of supported compilers includes gnu, cray, ibm, intel, llvm, and pgi. One must also set the `DIM` variable to either 1, 2, or 3, depending on the dimensionality of the problem.

Variables `DEBUG`, `USE_MPI` and `USE_OMP` are optional with default set to `TRUE`, `FALSE` and `FALSE`, respectively. The meaning of these variables should be obvious. When `DEBUG = TRUE`, aggressive compiler optimization flags are turned off and assertions in source code are turned on. For production runs, `DEBUG` should be set to `FALSE`.

After defining these make variables, a number of files, `Make.defs`, `Make.package` and `Make.rules`, are included in the `GNUmakefile`. AMReX-based applications do not need to include all directories in AMReX; an application which does not use particles, for example, does not need to include files from the Particle directory in its build. In this simple example, we only need to include `$ (AMREX_HOME) /Src/Base/Make.package`. An application code also has its own `Make.package` file (e.g., `./Make.package` in this example) to append source files to the build system using operator `+=`. Variables for various source files are shown below.

CExE_sources C++ source files. Note that C++ source files are assumed to have a `.cpp` extension.

CExE_headers C++ headers with `.h` or `.H` extension.

cExE_sources C source files with `.c` extension.

cExE_headers C headers with `.h` extension.

f90ExE_sources Free format Fortran source with `.f90` extension.

F90ExE_sources Free format Fortran source with `.F90` extension. Note that these Fortran files will go through preprocessing.

In this simple example, the extra source file, `main.cpp` is in the current directory that is already in the build system's search path. If this example has files in a subdirectory (e.g., `mysrcdir`), you will then need to add the following to `Make.package`.

```
VPATH_LOCATIONS += mysrcdir
INCLUDE_LOCATIONS += mysrcdir
```

Here `VPATH_LOCATIONS` and `INCLUDE_LOCATIONS` are the search path for source and header files, respectively.

3.1.2 Tweaking the Make System

The GNU Make build system is located at `amrex/Tools/GNUMake`. You can read `README.md` and the `make` files there for more information. Here we will give a brief overview.

Besides building executable, other common `make` commands include:

make clean This removes the executable, `.o` files, and the temporarily generated files. Note that one can add additional targets to this rule using the double colon (`::`)

make realclean This removes all files generated by `make`.

make help This shows the rules for compilation.

make print-xxx This shows the value of variable `xxx`. This is very useful for debugging and tweaking the make system.

Compiler flags are set in `amrex/Tools/GNUMake/comps/`. Note that variables like `CC` and `CFLAGS` are reset in that directory and their values in environment variables are disregarded. Site-specific setups (e.g., the MPI installation) are in `amrex/Tools/GNUMake/sites/`, which includes a generic setup in `Make.unknown`. You can override the setup by having your own `sites/Make.$(host_name)` file, where variable `host_name` is your host name in the make system and can be found via `make print-host_name`. You can also have an `amrex/Tools/GNUMake/Make.local` file to override various variables. See `amrex/Tools/GNUMake/Make.local.template` for more examples of how to customize the build process.

3.1.3 Specifying your own compiler

The `amrex/Tools/GNUMake/Make.local` file can also specify your own compile commands by setting the variables `CXX`, `CC`, `FC`, and `F90`. This might be necessary if your system contains non-standard names for compiler commands.

For example, the following `amrex/Tools/GNUMake/Make.local` builds AMReX using a specific compiler (in this case `gcc-8`) without MPI. Whenever `USE_MPI` is true, this configuration defaults to the appropriate `mpicxxx` command:

```
ifeq ($USE_MPI, TRUE)
  CXX = mpicxx
  CC = mpicc
  FC = mpif90
  F90 = mpif90
else
  CXX = g++-8
  CC = gcc-8
  FC = gfortran-8
  F90 = gfortran-8
endif
```

For building with MPI, we assume `mpicxx`, `mpif90`, etc. provide access to the correct underlying compilers.

3.1.4 GCC on macOS

The example configuration above should also run on the latest macOS. On macOS the default cxx compiler is clang, whereas the default fortran compiler is gfortran. Sometimes it is good to avoid mixing compilers, in that case we can use the `Make.local` to force using GCC. However, macOS' Xcode ships with its own (woefully outdated) version of GCC (4.2.1). It is therefore recommended to install GCC using the `homebrew` package manager. Running `brew install gcc` installs gcc with names reflecting the version number. If GCC 8.2 is installed, homebrew installs it as `gcc-8`. AMReX can be built using `gcc-8` (with and without MPI) by using the following `amrex/Tools/GNUMake/Make.local`:

```
CXX = g++-8
CC = gcc-8
FC = gfortran-8
F90 = gfortran-8

INCLUDE_LOCATIONS += /usr/local/include
```

The additional `INCLUDE_LOCATIONS` are installed using homebrew also. Note that if you are building AMReX using homebrew's gcc, it is recommended that you use homebrew's mpich. Normally it is fine to simply install its binaries: `brew install mpich`. But if you are experiencing problems, we suggest building mpich using homebrew's gcc: `brew install mpich --cc=gcc-8`.

3.2 Building libamrex

If an application code already has its own elaborated build system and wants to use AMReX as an external library, this might be your choice. In this approach, one runs `./configure`, followed by `make` and `make install`. Other `make` options include `make distclean` and `make uninstall`. In the top AMReX directory, one can run `./configure -h` to show the various options for the `configure` script. This approach is built on the AMReX GNU Make system. Thus the section on *Building with GNU Make* is recommended if any fine tuning is needed. The result of `./configure` is `GNUmakefile` in the AMReX top directory. One can modify the `make` file for fine tuning.

3.3 Building with CMake

An alternative to the approach described in the section on [Building libamrex](#) is to install AMReX as an external library by using the CMake build system. A CMake build is a two-step process. First `cmake` is invoked to create configuration files and makefiles in a chosen directory (`builddir`). This is roughly equivalent to running `./configure` (see the section on [Building libamrex](#)). Next, the actual build and installation are performed by invoking `make install` from within `builddir`. This installs the library files in a chosen installation directory (`installdir`). If no installation path is provided by the user, AMReX will be installed in `/path/to/amrex/installdir`. The CMake build process is summarized as follows:

```
mkdir /path/to/builddir
cd /path/to/builddir
cmake [options] -DCMAKE_INSTALL_PREFIX:PATH=/path/to/installdir /path/to/amrex
make install
```

In the above snippet, `[options]` indicates one or more options for the customization of the build, as described in the subsection on [Customization options](#). Although the AMReX source could be used as build directory, we advise against doing so. After the installation is complete, `builddir` can be removed.

3.3.1 Cmake and macOS

You can also specify your own compiler in `cmake` using the `-DCMAKE_C_COMPILER` and `-DCMAKE_CXX_COMPILER` options. While not strictly necessary when using homebrew on macOS, it is highly recommended that the user specifies `-DCMAKE_C_COMPILER=$` (which `gcc-X`) `-DCMAKE_CXX_COMPILER=$` (which `g++-X`) (where `X` is the GCC version installed by homebrew) when using `gfortran`. This is because homebrew's `cmake` defaults to the clang c/c++ compiler. Normally clang plays well with `gfortran`, but if there are some issues, we recommend telling `cmake` to use `gcc` for c/c++ also.

3.3.2 Customization options

AMReX configuration settings may be specified on the command line with the `-D` option. For example, one can enable OpenMP support as follows:

```
cmake -DENABLE_OMP=1 -DCMAKE_INSTALL_PREFIX:PATH=/path/to/installdir /path/to/amrex
```

The list of available option is reported in the table on [AMReX build options](#) below.

Table 3.2: AMReX build options

| Option Name | Description | De-fault | Possible values |
|------------------------------|--|----------|-----------------|
| DEBUG | Build AMReX in debug mode | OFF | ONE, OFF |
| DIM | Dimension of AMReX build | 3 | 2, 3 |
| ENABLE_DP | Build with double-precision reals | ON | ON, OFF |
| ENABLE_PIC | Build Position Independent Code | OFF | ON, OFF |
| ENABLE_MPI | Build with MPI support | ON | ON OFF |
| ENABLE_OMP | Build with OpenMP support | OFF | ON, OFF |
| ENABLE_FORTRAN_INTERFACES | Build Fortran API | ON | ON, OFF |
| ENABLE_LINEAR_SOLVERS | Build AMReX linear solvers | ON | ON, OFF |
| ENABLE_LINEAR_SOLVERS_LEGACY | Build AMReX linear solvers (legacy components) | ON | ON, OFF |
| ENABLE_FBASELIB | Build (deprecated) Fortran kernel | ON | ON, OFF |
| ENABLE_AMRDATA | Build data services | OFF | ON, OFF |
| ENABLE PARTICLES | Build particle classes | OFF | ON OFF |
| ENABLE_DP PARTICLES | Use double-precision reals in particle classes | ON | ON, OFF |
| ENABLE_BASE_PROFILE | Build with basic profiling support | OFF | ON, OFF |
| ENABLE_TINY_PROFILE | Build with tiny profiling support | OFF | ON, OFF |
| ENABLE_TRACE_PROFILE | Build with trace-profiling support | OFF | ON, OFF |
| ENABLE_COMM_PROFILE | Build with comm-profiling support | OFF | ON, OFF |
| ENABLE_MEM_PROFILE | Build with memory-profiling support | OFF | ON, OFF |
| ENABLE_PROFPARSER | Build with profile parser support | OFF | ON, OFF |
| ENABLE_BACKTRACE | Build with backtrace support | OFF | ON, OFF |
| ENABLE_FPE | Build with Floating Point Exceptions checks | OFF | ON, OFF |
| ENABLE ASSERTIONS | Build with assertions turned on | OFF | ON, OFF |
| CMAKE_Fortran_FLAGS | User-defined Fortran flags | | user-defined |
| CMAKE_CXX_FLAGS | User-defined C++ flags | | user-defined |
| ENABLE_3D_NODAL_MGML | Enable 3D nodal projection | OFF | ON, OFF |
| ALGOIM_INSTALL_DIR | Path to Algoim installation directory | | user-defined |
| BLITZ_INSTALL_DIR | Path to Blitz installation directory | | user-defined |

The option `ENABLE_LINEAR_SOLVERS=ON` triggers the inclusion of C++-based linear solvers in the build. Fortran-based linear solvers can be included as well by providing the option `ENABLE_FBASELIB=ON` in addition to `ENABLE_LINEAR_SOLVERS=ON`.

The option `DEBUG=ON` implies `ENABLE_ASSERTION=ON`. In order to turn off assertions in debug mode, `ENABLE_ASSERTION=OFF` must be set explicitly while invoking CMake.

The options `CMAKE_Fortran_FLAGS` and `CMAKE_CXX_FLAGS` allow the user to set his own compilation flags for Fortran and C++ source files respectively. If `CMAKE_Fortran_FLAGS`/`CMAKE_CXX_FLAGS` are not set by the user, they will be initialized with the value of the environmental variables `FFLAGS`/`CXXFLAGS`. If `FFLAGS`/`CXXFLAGS` are not defined in the environment, `CMAKE_Fortran_FLAGS`/`CMAKE_CXX_FLAGS` will be set to the AMReX default values defined in `/path/to/amrex/Tools/CMake/AMReX_Compilers.cmake`.

The option `ENABLE_3D_NODAL_MGML` enables AMReX 3D nodal projection. This option requires two external libraries: Blitz and Algoim. The user can provide the location of both libraries via `BLITZ_INSTALL_DIR` and `ALGOIM_INSTALL_DIR`. However, if one or both of these options is not provided, AMReX will download and build Blitz and/or Algoim automatically. It should be noted that AMReX 2D nodal projection does not require the use of external libraries.

3.3.3 Importing AMReX into your CMake project

In order to import the AMReX library into your CMake project, you need to include the following line in the appropriate CMakeLists.txt file:

```
find_package (AMReX 18 [REQUIRED] [HINTS /path/to/installdir/] )
```

In the above snippet, 18 refer to the minimum AMReX version supporting the import feature discussed here. Linking AMReX to any target defined in your CMake project is done by including the following line in the appropriate CMakeLists.txt file

```
target_link_libraries ( <your-target-name> AMReX::amrex )
```

The above snippet will take care of properly linking <your-target-name> to AMReX and to all the required transitive dependencies.

**CHAPTER
FOUR**

BASICS

In this chapter, we present the basics of AMReX. The implementation source codes are in `amrex/Src/Base/`. Note that AMReX classes and functions are in namespace `amrex`. For clarity, we usually drop `amrex::` in the example codes here. It is also assumed that headers have been properly included. We recommend you study the tutorial in `amrex/Tutorials/Basic/HeatEquation_EX1_C` while reading this chapter. After reading this chapter, one should be able to develop single-level parallel codes using AMReX. It should also be noted that this is not a comprehensive reference manual.

4.1 Dimensionality

As we have mentioned in [Building AMReX](#), the dimensionality of AMReX must be set at compile time. A macro, `AMREX_SPACEDIM`, is defined to be the number of spatial dimensions. C++ codes can also use the `amrex::SpaceDim` variable. Fortran codes can use either the macro and preprocessing or do

```
use amrex_fort_module, only : amrex_spacedim
```

The coordinate directions are zero based.

4.2 Vector and Array

`Vector` class in `AMReX_Vector.H` is derived from `std::vector`. The main difference between `Vector` and `std::vector` is that `Vector::operator[]` provides bound checking when compiled with `DEBUG=TRUE`.

`Array` class in `AMReX_Array.H` is simply an alias to `std::array`.

4.3 Real

AMReX can be compiled to use either double precision (which is the default) or single precision. `amrex::Real` is typedef'd to either `double` or `float`. C codes can use `amrex_real`. They are defined in `AMReX_REAL.H`. The data type is accessible in Fortran codes via

```
use amrex_fort_module, only : amrex_real
```

4.4 ParallelDescriptor

AMReX users do not need to use MPI directly. Parallel communication is often handled by the data abstraction classes (e.g.,*MultiFab*; section on *FabArray*, *MultiFab* and *iMultiFab*). In addition, AMReX has provided namespace *ParallelDescriptor* in *AMReX_ParallelDescriptor.H*. The frequently used functions are

```
int myproc = ParallelDescriptor::MyProc(); // Return the rank

int nprocs = ParallelDescriptor::NProcs(); // Return the number of processes

if (ParallelDescriptor::IOProcessor()) {
    // Only the I/O process executes this
}

int ioproc = ParallelDescriptor::IOProcessorNumber(); // I/O rank

ParallelDescriptor::Barrier();

// Broadcast 100 ints from the I/O Processor
Vector<int> a(100);
ParallelDescriptor::Bcast(a.data(), a.size(),
                        ParallelDescriptor::IOProcessorNumber())

// See AMReX_ParallelDescriptor.H for many other Reduce functions
ParallelDescriptor::ReduceRealSum(x);
```

4.5 Print

AMReX provides classes in *AMReX_Print.H* for printing messages to standard output or any C++ ostream. The main reason one should use them instead of *std::cout* is that messages from multiple processes or threads do not get mixed up. Below are some examples.

```
Print() << "x = " << x << "\n"; // Print on I/O processor

Real pi = std::atan(1.0)*4.0;
// Print on rank 3 with precision of 17 digits
// SetPrecision does not modify cout's floating-point decimal precision setting.
Print(3).SetPrecision(17) << pi << "\n";

int oldprec = std::cout.precision(10);
Print() << pi << "\n"; // Print with 10 digits

AllPrint() << "Every process prints\n"; // Print on every process

std::ofstream ofs("my.txt", std::ofstream::out);
Print(ofs) << "Print to a file" << std::endl;
ofs.close();

AllPrintToFile("file.") << "Each process appends to its own file (e.g., file.3)\n";
```

4.6 ParmParse

ParmParse in AMReX_ParmParse.H is a class providing a database for the storage and retrieval of command-line and input-file arguments. When `amrex::Initialize(int& argc, char**& argv)` is called, the first command-line argument after the executable name (if there is one and it does not contain character =) is taken to be the inputs file, and the contents in the file are used to initialize the ParmParse database. The rest of the command-line arguments are also parsed by ParmParse. The format of the inputs file is a series of definitions in the form of `prefix.name = value value`. For each line, text after # are comments. Here is an example inputs file.

```
nsteps      = 100          # integer
nsteps      = 1000         # nsteps appears a second time
dt          = 0.03          # floating point number
ncells      = 128 64 32    # a list of 3 ints
xrange     = -0.5 0.5      # a list of 2 reals
title       = "Three Kingdoms" # a string
hydro.cfl   = 0.8          # with prefix, hydro
```

The following code shows how to use ParmParse to get/query the values.

```
ParmParse pp;

int nsteps = 0;
pp.query("nsteps", nsteps);
amrex::Print() << nsteps << "\n"; // 1000

Real dt;
pp.get("dt", dt); // runtime error if dt is not in inputs

Vector<int> numcells;
// The variable name 'numcells' can be different from parameter name 'ncells'.
pp.getarr("ncells", numcells);
amrex::Print() << numcells.size() << "\n"; // 3

Vector<Real> xr {-1.0, 1.0};
if (!queryarr("xrange", xr)) {
    amrex::Print() << "Cannot find xrange in inputs, "
    << "so the default {-1.0,1.0} will be used\n";
}

std::string title;
pp.query("title", title); // query string

ParmParse pph("hydro"); // with prefix 'hydro'
Real cfl;
pph.get("cfl", cfl); // get parameter with prefix
```

Note that when there are multiple definitions for a parameter ParmParse by default returns the last one. The difference between `query` and `get` should also be noted. It is a runtime error if `get` fails to get the value, whereas `query` returns an error code without generating a runtime error that will abort the run. If it is sometimes convenient to override parameters with command-line arguments without modifying the inputs file. The command-line arguments after the inputs file are added later than the file to the database and are therefore used by default. For example, one can run with

```
myexecutable myinputsfile ncells="64 32 16" hydro.cfl=0.9
```

to change the value of `ncells` and `hydro.cfl`.

4.7 Initialize and Finalize

As we have mentioned, `Initialize` must be called to initialize the execution environment for AMReX and `Finalize` must be paired with `Initialize` to release the resources used by AMReX. There are two versions of `Initialize`.

```
void Initialize (MPI_Comm mpi_comm,
                 std::ostream& a_osout = std::cout,
                 std::ostream& a_oserr = std::cerr);

void Initialize (int& argc, char***& argv, bool build_parm_parse=true,
                 MPI_Comm mpi_comm = MPI_COMM_WORLD,
                 const std::function<void()>& func_parm_parse = {},
                 std::ostream& a_osout = std::cout,
                 std::ostream& a_oserr = std::cerr);
```

`Initialize` tests if MPI has been initialized. If MPI has been initialized, AMReX will duplicate the `MPI_Comm` argument. If not, AMReX will initialize MPI and ignore the `MPI_Comm` argument.

Both versions have two optional `std::ostream` parameters, one for standard output in `Print` (section [Print](#)) and the other for standard error, and they can be accessed with functions `OutStream()` and `ErrorStream()`.

The first version of `Initialize` does not parse the command line options, whereas the second version will build `ParmParse` database (section [ParmParse](#)) unless `build_parm_parse` parameter is `false`. In the second version, one can pass a function that adds `ParmParse` parameters to the database instead of reading from command line or input file.

Because many AMReX classes and functions (including destructors inserted by the compiler) do not function properly after `amrex::Finalize` is called, it's best to put the codes between `amrex::Initialize` and `amrex::Finalize` into its scope (e.g., a pair of curly braces or a separate function) to make sure resources are properly freed.

4.8 Example of AMR Grids

In block-structured AMR, there is a hierarchy of logically rectangular grids. The computational domain on each AMR level is decomposed into a union of rectangular domains. Fig. 4.1 below shows an example of AMR with three total levels. In the AMReX numbering convention, the coarsest level is level 0. The coarsest grid (*black*) covers the domain with 16^2 cells. Bold lines represent grid boundaries. There are two intermediate resolution grids (*blue*) at level 1 and the cells are a factor of two finer than those at level 0. The two finest grids (*red*) are at level 2 and the cells are a factor of two finer than the level 1 cells. There are 1, 2 and 2 Boxes on levels 0, 1, and 2, respectively. Note that there is no direct parent-child connection. In this chapter, we will focus on single levels.

4.9 Box, IntVect and IndexType

`Box` in `AMReX_Box.H` is the data structure for representing a rectangular domain in indexing space. In Fig. 4.1, there are 1, 2 and 2 Boxes on levels 0, 1 and 2, respectively. `Box` is a dimension-dependent class. It has lower and upper corners (represented by `IntVect`) and an index type (represented by `IndexType`). A `Box` contains no floating-point data.

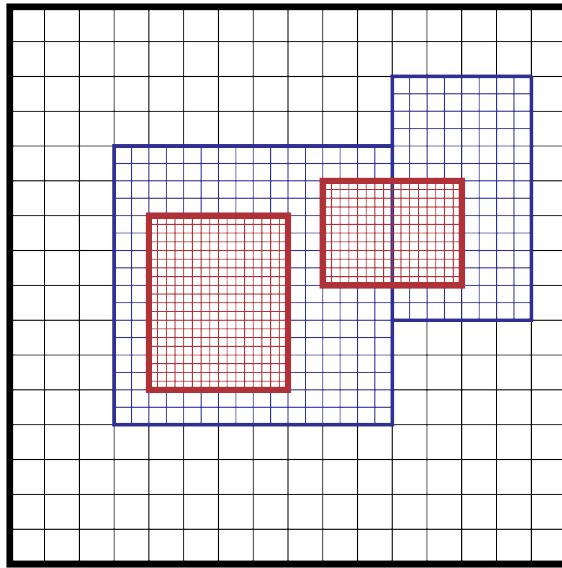


Fig. 4.1: Example of AMR grids. There are three levels in total. There are 1, 2 and 2 Boxes on levels 0, 1, and 2, respectively.

4.9.1 IntVect

`IntVect` is a dimension-dependent class representing an integer vector in `AMREXPACEDIM`-dimensional space. An `IntVect` can be constructed as follows,

```
IntVect iv(AMREX_D_DECL(19, 0, 5));
```

Here `AMREX_D_DECL` is a macro that expands `AMREX_D_DECL(19, 0, 5)` to either `19, 0, 5` or `19, 0, 0, 5` depending on the number of dimensions. The data can be accessed via `operator[]`, and the internal data pointer can be returned by function `getVect`. For example

```
for (int idim = 0; idim < AMREX_SPACEDIM; ++idim) {
    amrex::Print() << "iv[" << idim << "] = " << iv[idim] << "\n";
}
const int * p = iv.getVect(); // This can be passed to Fortran/C as an array
```

The class has a static function `TheZeroVector()` returning the zero vector, `TheUnitVector()` returning the unit vector, and `TheDimensionVector` (`int dir`) returning a reference to a constant `IntVect` that is zero except in the `dir`-direction. Note the direction is zero-based. `IntVect` has a number of relational operators, `==`, `!=`, `<`, `<=`, `>`, and `>=` that can be used for lexicographical comparison (e.g., key of `std::map`), and a class `IntVect::shift_hasher` that can be used as a hash function (e.g., for `std::unordered_map`). It also has various arithmetic operators. For example,

```
IntVect iv(AMREX_D_DECL(19, 0, 5));
IntVect iv2(AMREX_D_DECL(4, 8, 0));
iv += iv2; // iv is now (23, 8, 5)
iv *= 2;   // iv is now (46, 16, 10);
```

In AMR codes, one often needs to do refinement and coarsening on `IntVect`. The refinement operation can be done with the multiplication operation. However, the coarsening requires care because of the rounding towards zero behavior of integer division in Fortran, C and C++. For example `int i = -1/2` gives `i = 0`, and what we want is usually `i = -1`. Thus, one should use the coarsen functions:

```
IntVect iv(AMREX_D_DECL(127,127,127));
IntVect coarsening_ratio(AMREX_D_DECL(2,2,2));
iv.coarsen(2); // Coarsen each component by 2
iv.coarsen(coarsening_ratio); // Component-wise coarsening
const auto& iv2 = amrex::coarsen(iv, 2); // Return an IntVect w/o modifying iv
IntVect iv3 = amrex::coarsen(iv, coarsening_ratio); // iv not modified
```

Finally, we note that operator<< is overloaded for `IntVect` and therefore one can call

```
amrex::Print() << iv << "\n";
std::cout << iv << "\n";
```

4.9.2 IndexType

This class defines an index as being cell based or node based in each dimension. The default constructor defines a cell based type in all directions. One can also construct an `IndexType` with an `IntVect` with zero and one representing cell and node, respectively.

```
// Node in x-direction and cell based in y and z-directions
// (i.e., x-face of numerical cells)
IndexType xface(IntVect{AMREX_D_DECL(1,0,0)});
```

The class provides various functions including

```
// True if the IndexType is cell based in all directions.
bool cellCentered () const;

// True if the IndexType is cell based in dir-direction.
bool cellCentered (int dir) const;

// True if the IndexType is node based in all directions.
bool nodeCentered () const;

// True if the IndexType is node based in dir-direction.
bool nodeCentered (int dir) const;
```

Index type is a very important concept in AMReX. It is a way of representing the notion of indices i and $i + 1/2$.

4.9.3 Box

A `Box` is an abstraction for defining discrete regions of `AMREX_SPACEDIM`-dimensional indexing space. Boxes have an `IndexType` and two `IntVect`s representing the lower and upper corners. Boxes can exist in positive and negative indexing space. Typical ways of defining a `Box` are

```
IntVect lo(AMREX_D_DECL(64,64,64));
IntVect hi(AMREX_D_DECL(127,127,127));
IndexType typ({AMREX_D_DECL(1,1,1)});
Box cc(lo,hi); // By default, Box is cell based.
Box nd(lo,hi+1,typ); // Construct a nodal Box.
Print() << "A cell-centered Box " << cc << "\n";
Print() << "An all nodal Box " << nd << "\n";
```

Depending the dimensionality, the output of the code above is

```
A cell-centered Box ((64, 64, 64) (127, 127, 127) (0, 0, 0))
An all nodal Box   ((64, 64, 64) (128, 128, 128) (1, 1, 1))
```

For simplicity, we will assume it is 3D for the rest of this section. In the output, three integer tuples for each box are the lower corner indices, upper corner indices, and the index types. Note that 0 and 1 denote cell and node, respectively. For each tuple like $(64, 64, 64)$, the 3 numbers are for 3 directions. The two Boxes in the code above represent different indexing views of the same domain of 64^3 cells. Note that in AMReX convention, the lower side of a cell has the same integer value as the cell centered index. That is if we consider a cell based index represent i , the nodal index with the same integer value represents $i - 1/2$. Fig. 4.2 shows some of the different index types for 2D.



Fig. 4.2: Some of the different index types in two dimensions: (a) cell-centered, (b) x -face-centered (i.e., nodal in x -direction only), and (c) corner/nodal, i.e., nodal in all dimensions.

There are a number of ways of converting a Box from one type to another.

```
Box b0 ({64, 64, 64}, {127, 127, 127}); // Index type: (cell, cell, cell)

Box b1 = surroundingNodes(b0); // A new Box with type (node, node, node)
Print() << b1; // ((64, 64, 64) (128, 128, 128) (1, 1, 1))
Print() << b0; // Still ((64, 64, 64) (127, 127, 127) (0, 0, 0))

Box b2 = enclosedCells(b1); // A new Box with type (cell, cell, cell)
if (b2 == b0) { // Yes, they are identical.
    Print() << "b0 and b2 are identical!\n";
}

Box b3 = convert(b0, {0, 1, 0}); // A new Box with type (cell, node, cell)
Print() << b3; // ((64, 64, 64) (127, 128, 127) (0, 1, 0))

b3.convert({0, 0, 1}); // Convert b0 to type (cell, cell, node)
Print() << b3; // ((64, 64, 64) (127, 127, 128) (0, 0, 1))

b3.surroundingNodes(); // Exercise for you
b3.enclosedCells(); // Exercise for you
```

The internal data of Box can be accessed via various member functions. Examples are

```
const IntVect& smallEnd () const&; // Get the small end of the Box
int bigEnd (int dir) const; // Get the big end in dir direction
const int* loVect () const&; // Get a const pointer to the lower end
const int* hiVect () const&; // Get a const pointer to the upper end
```

Boxes can be refined and coarsened. Refinement or coarsening does not change the index type. Some examples are shown below.

```
Box ccbx ({16,16,16}, {31,31,31});
ccbx.refine(2);
Print() << ccbx; // ((32,32,32) (63,63,63) (0,0,0))
Print() << ccbx.coarsen(2); // ((16,16,16) (31,31,31) (0,0,0))

Box ndbx ({16,16,16}, {32,32,32}, {1,1,1});
ndbx.refine(2);
Print() << ndbx; // ((32,32,32) (64,64,64) (1,1,1))
Print() << ndbx.coarsen(2); // ((16,16,16) (32,32,32) (1,1,1))

Box facebx ({16,16,16}, {32,31,31}, {1,0,0});
facebx.refine(2);
Print() << facebx; // ((32,32,32) (64,63,63) (1,0,0))
Print() << facebx.coarsen(2); // ((16,16,16) (32,31,31) (1,0,0))

Box uncoarsenable ({16,16,16}, {30,30,30});
print() << uncoarsenable.coarsen(2); // ({8,8,8}, {15,15,15});
print() << uncoarsenable.refine(2); // ({16,16,16}, {31,31,31});
// Different from the original!
```

Note that the behavior of refinement and coarsening depends on the index type. A refined Box covers the same physical domain as the original Box, and a coarsened Box also covers the same physical domain if the original Box is coarsenable. Box uncoarsenable in the example above is considered uncoarsenable because its coarsened version does not cover the same physical domain in the AMR context.

Boxes can grow in one or all directions. There are a number of grow functions. Some are member functions of the Box class and others are free functions in the amrex namespace.

The Box class provides the following member functions testing if a Box or IntVect is contained within this Box. Note that it is a runtime error if the two Boxes have different types.

```
bool contains (const Box& b) const;
bool strictly_contains (const Box& b) const;
bool contains (const IntVect& p) const;
bool strictly_contains (const IntVect& p) const;
```

Another very common operation is the intersection of two Boxes like in the following examples.

```
Box b0 ({16,16,16}, {31,31,31});
Box b1 ({0, 0, 30}, {23,23,63});
if (b0.intersects(b1)) { // true
    Print() << "b0 and b1 intersect.\n";
}

Box b2 = b0 & b1; // b0 and b1 unchanged
Print() << b2; // ((16,16,30) (23,23,31) (0,0,0))

Box b3 = surroundingNodes(b0) & surroundingNodes(b1); // b0 and b1 unchanged
Print() << b3; // ((16,16,30) (24,24,32) (1,1,1))

b0 &= b2; // b2 unchanged
Print() << b0; // ((16,16,30) (23,23,31) (0,0,0))

b0 &= b3; // Runtime error because of type mismatch!
```

4.10 RealBox and Geometry

A RealBox stores the physical location in floating-point numbers of the lower and upper corners of a rectangular domain.

The Geometry class in AMReX_Geometry.H describes problem domain and coordinate system for rectangular problem domains. A Geometry object can be constructed with

```
explicit Geometry (const Box&      dom,
                  const RealBox* rb      = nullptr,
                  int          coord    = -1,
                  int*         is_per   = nullptr);
```

Here the constructor takes a cell-centered Box specifying the indexing space domain, an optional argument of RealBox pointer specifying the physical domain, an optional int specifying coordinate system type, and an optional int * specifying periodicity. If a RealBox is not given, AMReX will construct one based on ParmParse parameters, geometry.prob_lo and geometry.prob_hi, where each of the parameter is an array of AMREX_SPACEDIM real numbers. It's a runtime error if this fails. The optional argument for coordinate system is an integer type with valid values being 0 (Cartesian), or 1 (cylindrical), or 2 (spherical). If it is invalid as in the case of the default argument value, AMReX will query the ParmParse database for geometry.coord_sys and use it if one is found. If it cannot find the parameter, the coordinate system is set to 0 (i.e., Cartesian coordinates). The Geometry class has the concept of periodicity. An optional argument can be passed specifying periodicity in each dimension. If it is not given, the domain is assumed to be non-periodic unless there is the ParmParse integer array parameter geometry.is_periodic with 0 denoting non-periodic and 1 denoting periodic. Below is an example of defining a Geometry for a periodic rectangular domain of $[-1.0, 1.0]$ in each direction discretized with 64 numerical cells in each direction.

```
int n_cell = 64;

// This defines a Box with n_cell cells in each direction.
Box domain(IntVect{AMREX_D_DECL(      0,      0,      0)},
            IntVect{AMREX_D_DECL(n_cell-1, n_cell-1, n_cell-1)});

// This defines the physical box, [-1,1] in each direction.
RealBox real_box({AMREX_D_DECL(-1.0,-1.0,-1.0)},
                  {AMREX_D_DECL( 1.0, 1.0, 1.0)});

// This says we are using Cartesian coordinates
int coord = 0;

// This sets the boundary conditions to be doubly or triply periodic
Array<int,AMREX_SPACEDIM> is_periodic {AMREX_D_DECL(1,1,1)};

// This defines a Geometry object
Geometry geom(domain, &real_box, coord, is_periodic.data());
```

A Geometry object can return various information of the physical domain and the indexing space domain. For example,

```
const Real* problo = geom.ProbLo();           // Lower corner of the physical domain
Real yhi = geom.ProbHi(1);                   // y-direction upper corner
const Real* dx = geom.CellSize();             // Cell size for each direction
const Box& domain = geom.Domain();           // Index domain
bool is_per = Geometry::isPeriodic(0);        // Is periodic in x-direction?
if (Geometry::isAllPeriodic()) {}              // Periodic in all direction?
if (Geometry::isAnyPeriodic()) {}              // Periodic in any direction?
```

4.11 BoxArray

BoxArray is a class in AMReX_BoxArray.H for storing a collection of Boxes on a single AMR level. One can make a BoxArray out of a single Box and then chop it into multiple Boxes.

```
Box domain(IntVect{0,0,0}, IntVect{127,127,127});
BoxArray ba(domain); // Make a new BoxArray out of a single Box
Print() << "BoxArray size is " << ba.size() << "\n"; // 1
ba.setMaxSize(64); // Chop into boxes of 64^3 cells
Print() << ba;
```

The output is like below,

```
(BoxArray maxbox(8)
    m_ref->m_hash_sig(0)
((0,0,0) (63,63,63) (0,0,0)) ((64,0,0) (127,63,63) (0,0,0))
((0,64,0) (63,127,63) (0,0,0)) ((64,64,0) (127,127,63) (0,0,0))
((0,0,64) (63,63,127) (0,0,0)) ((64,0,64) (127,63,127) (0,0,0))
((0,64,64) (63,127,127) (0,0,0)) ((64,64,64) (127,127,127) (0,0,0)))
```

It shows that ba now has 8 Boxes, and it also prints out each Box.

In AMReX, BoxArray is a global data structure. It holds all the Boxes in a collection, even though a single process in a parallel run only owns some of the Boxes via domain decomposition. In the example above, a 4-process run may divide the work and each process owns say 2 Boxes (see section on [DistributionMapping](#)). Each process can then allocate memory for the floating point data on the Boxes it owns (see sections on [FabArray](#), [MultiFab](#) and [iMultiFab](#) & [BaseFab](#), [FArrayBox](#) and [IArrayBox](#)).

BoxArray has an indexing type, just like Box. Each Box in a BoxArray has the same type as the BoxArray itself. In the following example, we show how one can convert BoxArray to a different type.

```
BoxArray cellba(Box(IntVect{0,0,0}, IntVect{63,127,127}));
cellba.setMaxSize(64);
BoxArray faceba = cellba; // Make a copy
faceba.convert(IntVect{0,0,1}); // convert to index type (cell, cell, node)
// Return an all node BoxArray
const BoxArray& nodeba = amrex::convert(faceba, IntVect{1,1,1});
Print() << cellba[0] << "\n"; // ((0,0,0) (63,63,63) (0,0,0))
Print() << faceba[0] << "\n"; // ((0,0,0) (63,63,64) (0,0,1))
Print() << nodeba[0] << "\n"; // ((0,0,0) (64,64,64) (1,1,1))
```

As shown in the example above, BoxArray has an operator [] that returns a Box given an index. It should be emphasized that there is a difference between its behavior and the usual behavior of an subscript operator one might expect. The subscript operator in BoxArray returns by **value instead of reference**. This means code like below is meaningless because it modifies a temporary return value.

```
ba[3].coarsen(2); // DO NOT DO THIS! Doesn't do what one might expect.
```

BoxArray has a number of member functions that allow the Boxes to be modified. For example,

```
BoxArray& refine (int refinement_ratio); // Refine each Box in BoxArray
BoxArray& refine (const IntVect& refinement_ratio);
BoxArray& coarsen (int refinement_ratio); // Coarsen each Box in BoxArray
BoxArray& coarsen (const IntVect& refinement_ratio);
```

We have mentioned at the beginning of this section that BoxArray is a global data structure storing Boxes shared by all processes. The operation of a deep copy is thus undesirable because it is expensive and the extra copy wastes

memory. The implementation of the `BoxArray` class uses `std::shared_ptr` to an internal container holding the actual Box data. Thus making a copy of `BoxArray` is a quite cheap operation. The conversion of types and coarsening are also cheap because they can share the internal data with the original `BoxArray`. In our implementation, function `refine` does create a new deep copy of the original data. Also note that a `BoxArray` and its variant with a different type share the same internal data is an implementation detail. We discuss this so that the users are aware of the performance and resource cost. Conceptually we can think of them as completely independent of each other.

```
BoxArray ba(...); // original BoxArray
BoxArray ba2 = ba; // a copy that shares the internal data with the original
ba2.coarsen(2); // Modify the copy
// The original copy is unmodified even though they share internal data.
```

For advanced users, AMReX provides functions performing the intersection of a `BoxArray` and a `Box`. These functions are much faster than a naive implementation of performing intersection of the `Box` with each `Box` in the `BoxArray`. If one needs to perform those intersections, functions `amrex::intersect`, `BoxArray::intersects` and `BoxArray::intersections` should be used.

4.12 DistributionMapping

`DistributionMapping` is a class in `AMReX_DistributionMapping.H` that describes which process owns the data living on the domains specified by the Boxes in a `BoxArray`. Like `BoxArray`, there is an element for each `Box` in `DistributionMapping`, including the ones owned by other parallel processes. One can construct a `DistributionMapping` object given a `BoxArray`,

```
DistributionMapping dm {ba};
```

or by simply making a copy,

```
DistributionMapping dm {another_dm};
```

Note that this class is built using `std::shared_ptr`. Thus making a copy is relatively cheap in terms of performance and memory resources. This class has a subscript operator that returns the process ID at a given index.

By default, `DistributionMapping` uses an algorithm based on space filling curve to determine the distribution. One can change the default via the `ParmParse` parameter `DistributionMapping.strategy`. `KNAPSACK` is a common choice that is optimized for load balance. One can also explicitly construct a distribution. The `DistributionMapping` class allows the user to have complete control by passing an array of integers that represent the mapping of grids to processes.

```
DistributionMapping dm; // empty object
Vector<int> pmap {...};
// The user fills the pmap array with the values specifying owner processes
dm.define(pmap); // Build DistributionMapping given an array of process IDs.
```

4.13 BaseFab, FArrayBox and IArrayBox

AMReX is a block-structured AMR framework. Although AMR introduces irregularity to the data and algorithms, there is regularity at the block/`Box` level because each is still logically rectangular, and the data structure at the `Box` level is conceptually simple. `BaseFab` is a class template for multi-dimensional array-like data structure on a `Box`. The template parameter is typically basic types such as `Real`, `int` or `char`. The dimensionality of the array is `AMREX_SPACEDIM plus one`. The additional dimension is for the number of components. The data are internally stored in a contiguous block of memory in Fortran array order (i.e., column-major order) for

(x, y, z , component), and each component also occupies a contiguous block of memory because of the ordering. For example, a `BaseFab<Real>` with 4 components defined on a three-dimensional `Box(IntVect{-4, 8, 32}, IntVect{32, 64, 48})` is like a Fortran array of `real(amrex_real)`, dimension ($-4:32, 8:64, 32:48, 0:3$). Note that the convention in C++ part of AMReX is the component index is zero based. The code for constructing such an object is as follows,

```
Box bx(IntVect{-4, 8, 32}, IntVect{32, 64, 48});  
int numcomps = 4;  
BaseFab<Real> fab(bx, numcomps);
```

Most applications do not use `BaseFab` directly, but utilize specialized classes derived from `BaseFab`. The most common types are `FArrayBox` in `AMReX_FArrayBox.H` derived from `BaseFab<Real>` and `IArrayBox` in `AMReX_IArrayBox.H` derived from `BaseFab<int>`.

These derived classes also obtain many `BaseFab` member functions via inheritance. We now show some common usages of these functions. To get the `Box` where a `BaseFab` or its derived object is defined, one can call

```
const Box& box() const;
```

To the number of component, one can call

```
int nComp() const;
```

To get a pointer to the array data, one can call

```
T* dataPtr(int n=0); // Data pointer to the nth component  
// T is template parameter (e.g., Real)  
const T* dataPtr(int n=0) const; // const version
```

The typical usage of the returned pointer is then to pass it to a Fortran or C function that works on the array data (see the section on *Fortran, C and C++ Kernels*). `BaseFab` has several functions that set the array data to a constant value. Two examples are as follows.

```
void setVal(T x); // Set all data to x  
// Set the sub-region specified by bx to value x starting from component  
// nstart. ncomp is the total number of component to be set.  
void setVal(T x, const Box& bx, int nstart, int ncomp);
```

One can copy data from one `BaseFab` to another.

```
BaseFab<T>& copy (const BaseFab<T>& src, const Box& srcbox, int srccomp,  
const Box& destbox, int destcomp, int numcomp);
```

Here the function copies the data from the region specified by `srcbox` in the source `BaseFab src` into the region specified by `destbox` in the destination `BaseFab` that invokes the function call. Note that although `srcbox` and `destbox` may be different, they must be the same size, shape and index type, otherwise a runtime error occurs. The user also specifies how many components (`int numcomp`) are copied starting at component `srccomp` in `src` and stored starting at component `destcomp`. `BaseFab` has functions returning the minimum or maximum value.

```
T min (int comp=0) const; // Minimum value of given component.  
T min (const Box& subbox, int comp=0) const; // Minimum value of given  
// component in given subbox.  
T max (int comp=0) const; // Maximum value of given component.  
T max (const Box& subbox, int comp=0) const; // Maximum value of given  
// component in given subbox.
```

`BaseFab` also has many arithmetic functions. Here are some examples using `FArrayBox`.

```

Box box(IntVect{0,0,0}, IntVect{63,63,63});
int ncomp = 2;
FArrayBox fab1(box, ncomp);
FArrayBox fab2(box, ncomp);
fab1.setVal(1.0); // Fill fab1 with 1.0
fab1.mult(10.0, 0); // Multiply component 0 by 10.0
fab2.setVal(2.0); // Fill fab2 with 2.0
Real a = 3.0;
fab2.saxpy(a, fab1); // For both components, fab2 <- a * fab1 + fab2

```

For more complicated expressions that are not supported, one can write Fortran or C functions for those (see the section on [Fortran, C and C++ Kernels](#)). Note that BaseFab does provide operators for accessing the data directly in C++. For example, the `saxpy` example above can be done with

```

// Iterate over all components
for (int icomp=0; icomp < fab1.nComp(); ++icomp) {
    // Iterate over all cells in Box
    for (BoxIterator bit(fab1.box()); bit.ok(); ++bit) {
        // bit() returns IntVect
        fab2(bit(),icomp) = a * fab1(bit(),icomp) + fab2(bit(),icomp);
    }
}

```

But this approach is generally not recommended for performance reasons. However, it can be handy for debugging.

BaseFab and its derived classes are containers for data on `Box`. Recall that `Box` has various types (see the section on [Box, IntVect and IndexType](#)). The examples in this section so far use the default cell based type. However, some functions will result in a runtime error if the types mismatch. For example,

```

Box ccbx ({16,16,16}, {31,31,31});           // cell centered box
Box ndbx ({16,16,16}, {31,31,31}, {1,1,1}); // nodal box
FArrayBox ccfab(ccbx);
FArrayBox ndfbab(ndbx);
ccfab.setVal(0.0);
ndfbab.copy(ccfab); // runtime error due to type mismatch

```

Because it typically contains a lot of data, BaseFab's copy constructor and copy assignment operator are disabled to prevent performance degradation. However, BaseFab does provide a move constructor. In addition, it also provides a constructor for making an alias of an existing object. Here is an example using `FArrayBox`.

```

FArrayBox orig_fab(box, 4); // 4-component FArrayBox
// Make a 2-component FArrayBox that is an alias of orig_fab
// starting from component 1.
FArrayBox alias_fab(orig_fab, amrex::make_alias, 1, 2);

```

In this example, the alias `FArrayBox` has only two components even though the original one has four components. The alias has a sliced component view of the original `FArrayBox`. This is possible because of the array ordering. However, it is not possible to slice in the real space (i.e., the first `AMREX_SPACEDIM` dimensions). Note that no new memory is allocated in constructing the alias and the alias contains a non-owning pointer. It should be emphasized that the alias will contain a dangling pointer after the original `FArrayBox` reaches its end of life.

4.14 FabArray, MultiFab and iMultiFab

`FabArray<FAB>` is a class template in `AMReX_FabArray.H` for a collection of FABs on the same AMR level associated with a `BoxArray` (see the section on [BoxArray](#)). The template parameter `FAB` is usually `BaseFab<T>`

or its derived classes (e.g., `FArrayBox`). However, `FabArray` can also be used to hold other data structures. To construct a `FabArray`, a `BoxArray` must be provided because the `FabArray` is intended to hold *grid* data defined on a union of rectangular regions embedded in a uniform index space. For example, a `FabArray` object can be used to hold data for one level as in Fig. 4.1.

`FabArray` is a parallel data structure that the data (i.e., `FAB`) are distributed among parallel processes. For each process, a `FabArray` contains only the `FAB` objects owned by that process, and the process operates only on its local data. For operations that require data owned by other processes, remote communications are involved. Thus, the construction of a `FabArray` requires a `DistributionMapping` (see the section on *DistributionMapping*) that specifies which process owns which Box. For level 2 (*red*) in Fig. 4.1, there are two Boxes. Suppose there are two parallel processes, and we use a `DistributionMapping` that assigns one Box to each process. Then the `FabArray` on each process is built on the `BoxArray` with both Boxes, but contains only the `FAB` associated with its process.

In AMReX, there are some specialized classes derived from `FabArray`. The `iMultiFab` class in `AMReX_iMultiFab.H` is derived from `FabArray<IArryBox>`. The most commonly used `FabArray` kind class is `MultiFab` in `AMReX_MultiFab.H` derived from `FabArray<FArrayBox>`. In the rest of this section, we use `MultiFab` as example. However, these concepts are equally applicable to other types of `FabArrays`. There are many ways to define a `MultiFab`. For example,

```
// ba is BoxArray
// dm is DistributionMapping
int ncomp = 4;
int ngrow = 1;
MultiFab mf(ba, dm, ncomp, ngrow);
```

Here we define a `MultiFab` with 4 components and 1 ghost cell. A `MultiFab` contains a number of `FArrayBoxes` (see the section on *BaseFab*, *FArrayBox* and *IArryBox*) defined on Boxes grown by the number of ghost cells (1 in this example). That is the Box in the `FArrayBox` is not exactly the same as in the `BoxArray`. If the `BoxArray` has a `Box{ (7, 7, 7) (15, 15, 15) }`, the one used for constructing `FArrayBox` will be `Box{ (8, 8, 8) (16, 16, 16) }` in this example. For cells in `FArrayBox`, we call those in the original Box **valid cells** and the grown part **ghost cells**. Note that `FArrayBox` itself does not have the concept of ghost cells. Ghost cells are a key concept of `MultiFab`, however, that allows for local operations on ghost cell data originated from remote processes. We will discuss how to fill ghost cells with data from valid cells later in this section. `MultiFab` also has a default constructor. One can define an empty `MultiFab` first and then call the `define` function as follows.

```
MultiFab mf;
// ba is BoxArray
// dm is DistributionMapping
int ncomp = 4;
int ngrow = 1;
mf.define(ba, dm, ncomp, ngrow);
```

Given an existing `MultiFab`, one can also make an alias `MultiFab` as follows.

```
// orig_mf is an existing MultiFab
int start_comp = 3;
int num_comps = 1;
MultiFab alias_mf(orig_mf, amrex::make_alias, start_comp, num_comps);
```

Here the first integer parameter is the starting component in the original `MultiFab` that will become component 0 in the alias `MultiFab` and the second integer parameter is the number of components in the alias. It's a runtime error if the sum of the two integer parameters is greater than the number of the components in the original `MultiFab`. Note that the alias `MultiFab` has exactly the same number of ghost cells as the original `MultiFab`.

We often need to build new `MultiFab`s that have the same `BoxArray` and `DistributionMapping` as a given `MultiFab`. Below is an example of how to achieve this.

```
// mf0 is an already defined MultiFab
const BoxArray& ba = mf0.boxArray();
const DistributionMapping& dm = mf0.DistributionMap();
int ncomp = mf0.nComp();
int ngrow = mf0.nGrow();
MultiFab mf1(ba,dm,ncomp,ngrow); // new MF with the same ncomp and ngrow
MultiFab mf2(ba,dm,ncomp,0); // new MF with no ghost cells
// new MF with 1 component and 2 ghost cells
MultiFab mf3(mf0.boxArray(), mf0.DistributionMap(), 1, 2);
```

As we have repeatedly mentioned in this chapter that `Box` and `BoxArray` have various index types. Thus, `MultiFab` also has an index type that is obtained from the `BoxArray` used for defining the `MultiFab`. It should be noted again that index type is a very important concept in AMReX. Let's consider an example of a finite-volume code, in which the state is defined as cell averaged variables and the fluxes are defined as face averaged variables.

```
// ba is cell-centered BoxArray
// dm is DistributionMapping
int ncomp = 3; // Suppose the system has 3 components
int ngrow = 0; // no ghost cells
MultiFab state(ba, dm, ncomp, ngrow);
MultiFab xflux(amrex::convert(ba, IntVect{1,0,0}), dm, ncomp, 0);
MultiFab yflux(amrex::convert(ba, IntVect{0,1,0}), dm, ncomp, 0);
MultiFab zflux(amrex::convert(ba, IntVect{0,0,1}), dm, ncomp, 0);
```

Here all `MultiFab`s use the same `DistributionMapping`, but their `BoxArrays` have different index types. The state is cell-based, whereas the fluxes are on the faces. Suppose the cell based `BoxArray` contains a `Box{(8, 8, 16), (15, 15, 31)}`. The state on that `Box` is conceptually a Fortran Array with the dimension of `(8:15, 8:15, 16:31, 0:2)`. The fluxes are arrays with slightly different indices. For example, the *x*-direction flux for that `Box` has the dimension of `(8:16, 8:15, 16:31, 0:2)`. Note there is an extra element in *x*-direction.

The `MultiFab` class provides many functions performing common arithmetic operations on a `MultiFab` or between `MultiFab`s built with the *same* `BoxArray` and `DistributionMap`. For example,

```
Real dmin = mf.min(3); // Minimum value in component 3 of MultiFab mf
// no ghost cells included
Real dmax = mf.max(3,1); // Maximum value in component 3 of MultiFab mf
// including 1 ghost cell
mf.setVal(0.0); // Set all values to zero including ghost cells

MultiFab::Add(mfdst, mfsrc, sc, dc, nc, ng); // Add mfsrc to mfdst
MultiFab::Copy(mfdst, mfsrc, sc, dc, nc, ng); // Copy from mfsrc to mfdst
// MultiFab mfdst: destination
// MultiFab mfsrc: source
// int      sc   : starting component index in mfsrc for this operation
// int      dc   : starting component index in mfdst for this operation
// int      nc   : number of components for this operation
// int      ng   : number of ghost cells involved in this operation
//               mfdst and mfsrc may have more ghost cells
```

We refer the reader to `amrex/Src/Base/AMReX_MultiFab.H` and `amrex/Src/Base/AMReX_FabArray.H` for more details. It should be noted again it is a runtime error if the two `MultiFab`s passed to functions like `MultiFab::Copy` are not built with the *same* `BoxArray` (including index type) and `DistributionMapping`.

It is usually the case that the `Boxes` in the `BoxArray` used for building a `MultiFab` are non-intersecting except that they can be overlapping due to nodal index type. However, `MultiFab` can have ghost cells, and in that case `FArrayBoxes` are defined on `Boxes` larger than the `Boxes` in the `BoxArray`. Parallel communication is then needed

to fill the ghost cells with valid cell data from other FArrayBoxes possibly on other parallel processes. The function for performing this type of communication is `FillBoundary`.

```
MultiFab mf(...parameters omitted...);  
Geometry geom(...parameters omitted...);  
mf.FillBoundary(); // Fill ghost cells for all components  
// Periodic boundaries are not filled.  
mf.FillBoundary(geom.periodicity()); // Fill ghost cells for all components  
// Periodic boundaries are filled.  
mf.FillBoundary(2, 3); // Fill 3 components starting from component 2  
mf.FillBoundary(geom.periodicity(), 2, 3);
```

Note that `FillBoundary` does not modify any valid cells. Also note that `MultiFab` itself does not have the concept of periodic boundary, but `Geometry` has, and we can provide that information so that periodic boundaries can be filled as well. You might have noticed that a ghost cell could overlap with multiple valid cells from different FArrayBoxes in the case of nodal index type. In that case, it is unspecified that which valid cell's value is used to fill the ghost cell. It ought to be the case the values in those overlapping valid cells are the same up to roundoff errors. If a ghost cell does not overlap with any valid cells, its value will not be modified by `FillBoundary`.

Another type of parallel communication is copying data from one `MultiFab` to another `MultiFab` with a different `BoxArray` or the same `BoxArray` with a different `DistributionMapping`. The data copy is performed on the regions of intersection. The most generic interface for this is

```
mfdst.ParallelCopy(mfsrc, compsdc, compdst, ncomp, ngsrc, ngdst, period, op);
```

Here `mfdst` and `mfsrc` are destination and source `MultiFab`s, respectively. Parameters `compsdc`, `compdst`, and `ncomp` are integers specifying the range of components. The copy is performed on `ncomp` components starting from component `compsdc` of `mfsrc` and component `compdst` of `mfdst`. Parameters `ngsrc` and `ngdst` specify the number of ghost cells involved for the source and destination, respectively. Parameter `period` is optional, and by default no periodic copy is performed. Like `FillBoundary`, one can use `Geometry::periodicity()` to provide the periodicity information. The last parameter is also optional and is set to `FabArrayBase::COPY` by default. One could also use `FabArrayBase::ADD`. This determines whether the function copies or adds data from the source to the destination. Similar to `FillBoundary`, if a destination cell has multiple cells as source, it is unspecified that which source cell is used in `FabArrayBase::COPY`, and, for `FabArrayBase::ADD`, the multiple values are all added to the destination cell. This function has two variants, in which the periodicity and operation type are also optional.

```
mfdst.ParallelCopy(mfsrc, period, op); // mfdst and mfsrc must have the same  
// number of components  
mfdst.ParallelCopy(mfsrc, compsdc, compdst, ncomp, period, op);
```

Here the number of ghost cells involved is zero, and the copy is performed on all components if unspecified (assuming the two `MultiFab`s have the same number of components).

4.15 MFIter and Tiling

In this section, we will first show how `MFIter` works without tiling. Then we will introduce the concept of logical tiling. Finally we will show how logical tiling can be launched via `MFIter`.

4.15.1 MFIter without Tiling

In the section on [FabArray, MultiFab and iMultiFab](#), we have shown some of the arithmetic functionalities of `MultiFab`, such as adding two `MultiFab`s together. In this section, we will show how you can operate on the

MultiFab data with your own functions. AMReX provides an iterator, `MFIter` for looping over the FArrayBoxes in MultiFabs. For example,

```
for (MFIter mfi(mf); mfi.isValid(); ++mfi) // Loop over grids
{
    // This is the valid Box of the current FArrayBox.
    // By "valid", we mean the original ungrown Box in BoxArray.
    const Box& box = mfi.validbox();

    // A reference to the current FArrayBox in this loop iteration.
    FArrayBox& fab = mf[mfi];

    // Pointer to the floating point data of this FArrayBox.
    Real* a = fab.dataPtr();

    // This is the Box on which the FArrayBox is defined.
    // Note that "abox" includes ghost cells (if there are any),
    // and is thus larger than or equal to "box".
    const Box& abox = fab.box();

    // We can now pass the information to a function that does
    // work on the region (specified by box) of the data pointed to
    // by Real* a. The data should be viewed as multidimensional
    // with bounds specified by abox.
    // Function f1 has the signature of
    // void f1(const int*, const int*, Real*, const int*, const int*);
    f1(box.loVect(), box.hiVect(), a, abox.loVect(), abox.hiVect());
}
```

Here function `f1` is usually a Fortran subroutine with ISO C binding interface like below,

```
subroutine f1(lo, hi, a, alo, ahi) bind(c)
use amrex_fort_module, only : amrex_real
integer, intent(in) :: lo(3), hi(3), alo(3), ahi(3)
real(amrex_real),intent(inout)::a(alo(1):ahi(1),alo(2):ahi(2),alo(3):ahi(3))
integer :: i,j,k
do      k = lo(3), hi(3)
    do      j = lo(2), hi(2)
        do i = lo(1), hi(1)
            a(i,j,k) = ...
        end do
    end do
end do
end subroutine f1
```

Here `amrex_fort_module` is a Fortran module in AMReX and `amrex_real` is a Fortran kind parameter that matches `amrex::Real` in C++. In this example, we assumed the spatial dimension is 3. In 2D, the function interface is different. In the section on [Fortran, C and C++ Kernels](#), we will present a dimension-agnostic approach using macros provided by AMReX.

`MFIter` only loops over grids owned by this process. For example, suppose there are 5 Boxes in total and processes 0 and 1 own 2 and 3 Boxes, respectively. That is the MultiFab on process 0 has 2 FArrayBoxes, whereas there are 3 FArrayBoxes on process 1. Thus the numbers of iterations of `MFIter` are 2 and 3 on processes 0 and 1, respectively.

In the example above, MultiFab is assumed to have a single component. If it has multiple components, we can call `int nc = mf.nComp()` to get the number of components and pass `nc` to the kernel function.

There is only one MultiFab in the example above. Below is an example of working with multiple MultiFabs. Note that these two MultiFabs are not necessarily built on the same `BoxArray`. But they must have the same

DistributionMapping, and their BoxArrays are typically related (e.g., they are different due to index types).

```
// U and F are MultiFabs
int ncU = U.nComp();    // number of components
int ncF = F.nComp();
for (MFIter mfi(F); mfi.isValid(); ++mfi) // Loop over grids
{
    const Box& box = mfi.validbox();

    const FArrayBox& ufab = U[mfi];
    FArrayBox& ffab = F[mfi];

    Real* up = ufab.dataPtr();
    Real* fp = ufab.dataPtr();

    const Box& ubox = ufab.box();
    const Box& fbox = ffab.box();

    // Function f2 has the signature of
    // void f2(const int*, const int*,
    //          const Real*, const int*, const int*, const int*
    //          Real*, const int*, const int*, const int*);
    // This will compute f using u as inputs.
    f2(box.loVect(), box.hiVect(),
        up, ubox.loVect(), ubox.hiVect(), &ncU,
        fp, fbox.loVect(), fbox.hiVect(), &ncF);
}
```

Here again function f2 is usually a Fortran subroutine with ISO C binding interface like below,

```
subroutine f2(lo, hi, u, ulo, uhi, nu, f, flo, fhi, nf) bind(c)
use amrex_fort_module, only : amrex_real
integer, intent(in) :: lo(3),hi(3),ulo(3),uhi(3),nu,flo(3),fhi(3),nf
real(amrex_real),intent(in    ):::u(ulo(1):uhi(1),ulo(2):uhi(2),ulo(3):uhi(3),nu)
real(amrex_real),intent(inout):::f(flo(1):fhi(1),flo(2):fhi(2),flo(3):fhi(3),nf)
integer :: i,j,k
do n = 1, nf
    do      k = lo(3), hi(3)
        do j = lo(2), hi(2)
            do i = lo(1), hi(1)
                f(i,j,k,n) = ... u(...) ...
            end do
        end do
    end do
end subroutine f2
```

4.15.2 MFilter with Tiling

Tiling, also known as cache blocking, is a well known loop transformation technique for improving data locality. This is often done by transforming the loops into tiling loops that iterate over tiles and element loops that iterate over the data elements within a tile. For example, the original loops might look like

```
do k = kmin, kmax
    do j = jmin, jmax
        do i = imin, imax
```

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```

A(i,j,k) = B(i+1,j,k)+B(i-1,j,k)+B(i,j+1,k)+B(i,j-1,k) &
           +B(i,j,k+1)+B(i,j,k-1)-6.0d0*B(i,j,k)
end do
end do
end do

```

And the manually tiled loops might look like

```

jblocksize = 11
kblocksize = 16
jblocks = (jmax-jmin+jblocksize-1)/jblocksize
kblocks = (kmax-kmin+kblocksize-1)/kblocksize
do kb = 0, kblocks-1
  do jb = 0, jblocks-1
    do k = kb*kblocksize, min((kb+1)*kblocksize-1,kmax)
      do j = jb*jblocksize, min((jb+1)*jblocksize-1,jmax)
        do i = imin, imax
          A(i,j,k) = B(i+1,j,k)+B(i-1,j,k)+B(i,j+1,k)+B(i,j-1,k) &
                      +B(i,j,k+1)+B(i,j,k-1)-6.0d0*B(i,j,k)
        end do
      end do
    end do
  end do
end do
end do

```

As we can see, to manually tile individual loops is very labor-intensive and error-prone for large applications. AMReX has incorporated the tiling construct into `MFIter` so that the application codes can get the benefit of tiling easily. An `MFIter` loop with tiling is almost the same as the non-tiling version. The first example in (see the previous section on *MFIter without Tiling*) requires only two minor changes:

1. passing `true` when defining `MFIter` to indicate tiling;
2. calling `tilebox` instead of `validbox` to obtain the work region for the loop iteration.

```

// * true * turns on tiling
for (MFIter mfi(mf,true); mfi.isValid(); ++mfi) // Loop over tiles
{
  // tilebox() instead of validbox()
  const Box& box = mfi.tilebox();

  FArrayBox& fab = mf[mfi];
  Real* a = fab.dataPtr();
  const Box& abox = fab.box();

  f1(box.loVect(), box.hiVect(), a, abox.loVect(), abox.hiVect());
}

```

The second example in the previous section on *MFIter without Tiling* also requires only two minor changes.

```

// * true * turns on tiling
for (MFIter mfi(F,true); mfi.isValid(); ++mfi) // Loop over tiles
{
  // tilebox() instead of validbox()
  const Box& box = mfi.tilebox();

  const FArrayBox& ufab = U[mfi];
  FArrayBox& ffab = F[mfi];
}

```

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```

Real* up = ufab.dataPtr();
Real* fp = ufab.dataPtr();

const Box& ubox = ufab.box();
const Box& fbox = ffab.box();

f2(box.loVect(), box.hiVect(),
    up, ubox.loVect(), ubox.hiVect(), &ncU,
    fp, fbox.loVect(), fbox.hiVect(), &ncF);
}

```

The kernels functions like `f1` and `f2` in the two examples here usually require very little changes.

Table 4.1: Comparison of MFIter with (right) and without (left) tiling.

| | |
|--|---|
| | |
| <p>Example of cell-centered valid boxes. There are two valid boxes in this example. Each has 8^2 cells.</p> | <p>Example of cell-centered tile boxes. Each grid is <i>logically</i> broken into 4 tiles, and each tile as 4^2 cells. There are 8 tiles in total.</p> |

Table 4.1 shows an example of the difference between `validbox` and `tilebox`. In this example, there are two grids of cell-centered index type. The function `validbox` always returns a `Box` for the valid region of an `FArrayBox` no matter whether or not tiling is enabled, whereas the function `tilebox` returns a `Box` for a tile. (Note that when tiling is disabled, `tilebox` returns the same `Box` as `validbox`.) The number of loop iteration is 2 in the non-tiling version, whereas in the tiling version the kernel function is called 8 times.

The tile size can be explicitly set when defining `MFIter`.

```

// No tiling in x-direction. Tile size is 16 for y and 32 for z.
for (MFIter mfi(mf, IntVect(1024000, 16, 32)); mfi.isValid(); ++mfi) {...}

```

An `IntVect` is used to specify the tile size for every dimension. A tile size larger than the grid size simply means tiling is disable in that direction. AMReX has a default tile size `IntVect{1024000, 8, 8}` in 3D and no tiling in 2D. This is used when tile size is not explicitly set but the tiling flag is on. One can change the default size using `ParmParse` (section `ParmParse`) parameter `fabarray.mfiter_tile_size`.

Table 4.2: Comparison of MFIter with (right) and without (left) tiling, for face-centered nodal indexing.

| | |
|--|---|
| | |
| <p>Example of face valid boxes. There are two valid boxes in this example. Each has 9×8 points. Note that points in one Box may overlap with points in the other Box. However, the memory locations for storing floating point data of those points do not overlap, because they belong to separate FArrayBoxes.</p> | <p>Example of face tile boxes. Each grid is logically broken into 4 tiles as indicated by the symbols. There are 8 tiles in total. Some tiles have 5×4 points, whereas others have 4×4 points. Points from different Boxes may overlap, but points from different tiles of the same Box do not.</p> |

Usually MFIter is used for accessing multiple MultiFabs like the second example, in which two MultiFabs, U and F, use MFIter via operator []. These different MultiFabs may have different BoxArrays. For example, U might be cell-centered, whereas F might be nodal in x -direction and cell in other directions. The MFIter::validbox and tilebox functions return Boxes of the same type as the MultiFab used in defining the MFIter (F in this example). Table 4.2 illustrates an example of non-cell-centered valid and tile boxes. Besides validbox and tilebox, MFIter has a number of functions returning various Boxes. Examples include,

```
Box fabbox() const;           // Return the Box of the FArrayBox

// Return grown tile box. By default it grows by the number of
// ghost cells of the MultiFab used for defining the MFIter.
Box growntilebox(int ng=-1000000) const;

// Return tilebox with provided nodal flag as if the MFIter
// is constructed with MultiFab of such flag.
Box tilebox(const IntVect& nodal_flag);
```

It should be noted that the function growntilebox does not grow the tile Box like a normal Box. Growing a Box normally means the Box is extended in every face of every dimension. However, the function growntilebox only extends the tile Box in such a way that tiles from the same grid do not overlap. This is the basic design principle of these various tiling functions. Tiling is a way of domain decomposition for work sharing. Overlapping tiles is undesirable because work would be wasted and for multi-threaded codes race conditions could occur.

Table 4.3: Comparing growing cell-type and face-type tile boxes.

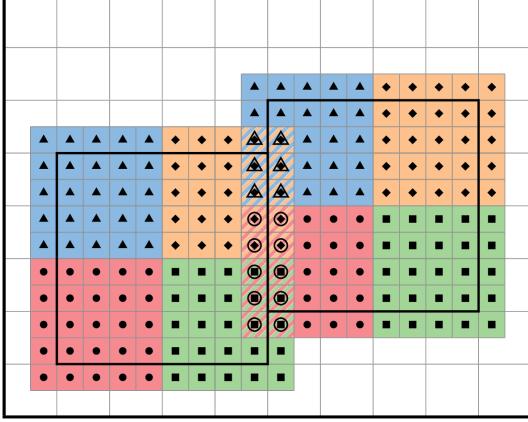
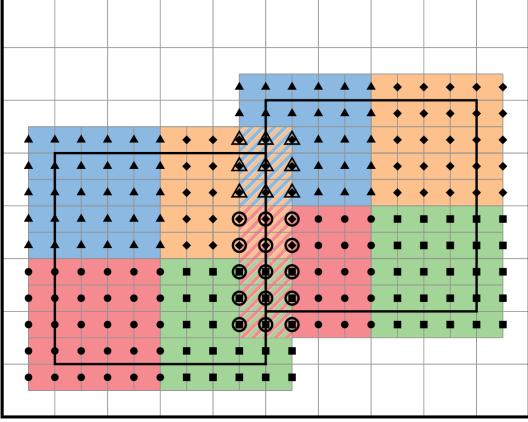
| | |
|---|---|
|  |  |
| Example of cell-centered grown tile boxes. As indicated by symbols, there are 8 tiles and four in each grid in this example. Tiles from the same grid do not overlap. But tiles from different grids may overlap. | Example of face type grown tile boxes. As indicated by symbols, there are 8 tiles and four in each grid in this example. Tiles from the same grid do not overlap even though they have face index type. |

Table 4.3 illustrates an example of `growntilebox`. These functions in `MFIter` return `Box` by value. There are three ways of using these functions.

```
const Box& bx = mfi.validbox(); // const& to temporary object is legal

// Make a copy if Box needs to be modified later.
// Compilers can optimize away the temporary object.
Box bx2 = mfi.validbox();
bx2.surroundingNodes();

Box&& bx3 = mfi.validbox(); // bound to the return value
bx3.enclosedCells();
```

But `Box& bx = mfi.validbox()` is not legal and will not compile.

4.16 Fortran, C and C++ Kernels

In the section on [MFIter and Tiling](#), we have shown that a typical pattern for working with MultiFab is to use `MFIter` to iterate over the data. In each iteration, a kernel function is called to work on the data and the work region is specified by a `Box`. When tiling is used, the work region is a tile. The tiling is logical in the sense that there is no data layout transformation. The kernel function still gets the whole arrays in `FArrayBoxes`, even though it is supposed to work on a tile region of the arrays. Fortran is often used for writing these kernels because of its native multi-dimensional array support. To C++, these kernel functions are C functions, whose function signatures are typically declared in a header file named `*_f.H` or `*_F.H`. We recommend the users to follow this convention. Examples of these function declarations are as follows.

```
#include <AMReX_BLFort.H>
#ifndef __cplusplus
```

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```

extern "C"
{
#endiff
    void f1(const int*, const int*, amrex_real*, const int*, const int*);
    void f2(const int*, const int*,  

            const amrex_real*, const int*, const int*, const int*  

            amrex_real*, const int*, const int*, const int*);
#ifdef __cplusplus
}
#endiff

```

One can write the functions in C and should include the header containing the function declarations in the C source code to ensure type safety. However, we typically write these kernel functions in Fortran because of the native multi-dimensional array support by Fortran. As we have seen in the section on [MFIter and Tiling](#), these Fortran functions take C pointers and view them as multi-dimensional arrays of the shape specified by the additional integer arguments. Note that Fortran takes arguments by reference unless the `value` keyword is used. So an integer argument on the Fortran side matches an integer pointer on the C++ side. Thanks to Fortran 2003, function name mangling is easily achieved by declaring the Fortran function as `bind(c)`.

AMReX provides many macros for passing an FArrayBox's data into Fortran/C. For example

```

for (MFIter mfi(mf,true); mfi.isValid(); ++mfi)
{
    const Box& box = mfi.tilebox();
    f(BL_TO_FORTRAN_BOX(box),
      BL_TO_FORTRAN_ANYD(mf[mfi]));
}

```

Here `BL_TO_FORTRAN_BOX` takes a `Box` and provides two `int *`'s specifying the lower and upper bounds of the `Box`. `BL_TO_FORTRAN_ANYD` takes an `FArrayBox` returned by `mf[mfi]` and the preprocessor turns it into `Real *, int *, int *`, where `Real *` is the data pointer that matches `real` array argument in Fortran, the first `int *` (which matches an integer argument in Fortran) specifies the lower bounds, and the second `int *` the upper bounds of the spatial dimensions of the array. Similar to what we have seen in the section on [MFIter and Tiling](#), a matching Fortran function is shown below,

```

subroutine f(lo, hi, u, ulo, uhi) bind(c)
  use amrex_fort_module, only : amrex_real
  integer, intent(in) :: lo(3),hi(3),ulo(3),uhi(3)
  real(amrex_real),intent(inout)::u(ulo(1):uhi(1),ulo(2):uhi(2),ulo(3):uhi(3))
end subroutine f

```

Here, the size of the integer arrays is 3, the maximal number of spatial dimensions. If the actual spatial dimension is less than 3, the values in the degenerate dimensions are set to zero. So the Fortran function interface does not have to change according to the spatial dimensionality, and the bound of the third dimension of the data array simply becomes `0:0`. With the data passed by `BL_TO_FORTRAN_BOX` and `BL_TO_FORTRAN_ANYD`, this version of Fortran function interface works for any spatial dimensions. If one wants to write a special version just for 2D and would like to use 2D arrays, one can use

```

subroutine f2d(lo, hi, u, ulo, uhi) bind(c)
  use amrex_fort_module, only : amrex_real
  integer, intent(in) :: lo(2),hi(2),ulo(2),uhi(2)
  real(amrex_real),intent(inout)::u(ulo(1):uhi(1),ulo(2):uhi(2))
end subroutine f2d

```

Note that this does not require any changes in the C++ part, because when C++ passes an integer pointer pointing to an array of three integers Fortran can treat it as a 2-element integer array.

Another commonly used macro is `BL_TO_FORTRAN`. This macro takes an `FArrayBox` and provides a real pointer for the floating point data array and a number of integer scalars for the bounds. However, the number of the integers depends on the dimensionality. More specifically, there are 6 and 4 integers for 2D and 3D, respectively. The first half of the integers are the lower bounds for each spatial dimension and the second half the upper bounds. For example,

```
subroutine f2d(u, ulo1, ulo2, uhi1, uhi2) bind(c)
  use amrex_fort_module, only : amrex_real
  integer, intent(in) :: ulo1, ulo2, uhi1, uhi2
  real(amrex_real),intent(inout)::u(ulo1:uhi1,ulo2:uhi2)
end subroutine f2d

subroutine f3d(u, ulo1, ulo2, ulo3, uhi1, uhi2, uhi3) bind(c)
  use amrex_fort_module, only : amrex_real
  integer, intent(in) :: ulo1, ulo2, ulo3, uhi1, uhi2, uhi3
  real(amrex_real),intent(inout)::u(ulo1:uhi1,ulo2:uhi2,ulo3:uhi3)
end subroutine f3d
```

Here for simplicity we have omitted passing the tile Box.

Usually `MultiFab`s have multiple components. Thus we often also need to pass the number of component into Fortran functions. We can obtain the number by calling the `MultiFab::nComp()` function, and pass it to Fortran as we have seen in the section on [MFIter and Tiling](#). We can also use the `BL_TO_FORTRAN_FAB` macro that is similar to `BL_TO_FORTRAN_ANYD` except that it provides an additional `int *` for the number of components. The Fortran function matching `BL_TO_FORTRAN_FAB(fab)` is then like below,

```
subroutine f(u, ulo, uhi,nu) bind(c)
  use amrex_fort_module, only : amrex_real
  integer, intent(in) :: lo(3),hi(3),ulo(3),uhi(3),nu
  real(amrex_real),intent(inout)::u(ulo(1):uhi(1),ulo(2):uhi(2),ulo(3):uhi(3),nu)
end subroutine f
```

There is a potential type safety issue when calling Fortran functions from C++. If there is a mismatch between the function declaration on the C++ side and the function definition in Fortran, the compiler cannot catch it. For example

```
// function declaration
extern "C" {
    void f (amrex_real* x);
}

for (MFIter mfi(mf,true); mfi.isValid(); ++mfi)
{
    f(mf[mfi].dataPtr());
}

! Fortra definition
subroutine f(x,y) bind(c)
    implicit none
    integer x, y
end subroutine f
```

The code above will compile without errors even though the number of arguments and types don't match.

To help detect this kind of issues, AMReX provides a type check tool. Note that it only works when GCC is used. In the directory an AMReX based code is compiled, type

```
make typecheck
```

Extra arguments used in a usual AMReX build (e.g., `USE_MPI=TRUE DIM=2`) can be added. When it finishes, the output may look like,

```
Function my_f in main_F.H vs. Fortran procedure in f.f90
  number of arguments 1 does NOT match 2.
  arg #1: C type ['double', 'pointer'] does NOT match Fortran type ('INTEGER 4',
  ↪'pointer', 'x').
22 functions checked, 1 error(s) found. More details can be found in tmp_build_dir/t/
↪3d.gnu.DEBUG.EXE/amrex_typecheck.ou.
```

It should be noted that Fortran by default passes argument by reference. In the example output above, `pointer` in Fortran type ('INTEGER 4', 'pointer', 'x') means it's a reference to argument (i.e., C pointer), not a Fortran pointer.

The type check tool has known limitations. For a function to be checked by the tool in the GNU make build system, the declaration must be in a header file named `*_f.H` or `*_F.H`, and the header file must be in the `CMAKE_HEADERS` make variable. The headers are preprocessed first by `cpp` as C language, and is then parsed by `pycparser` (<https://pypi.python.org/pypi/pycparser>) that needs to be installed on your system. Because `pycparser` is a C parser, C++ parts of the headers (e.g., `extern "C" {}`) need to be hidden with macro `#ifdef __cplusplus`. Headers like `AMReX_BLFort.H` can be used as a C header, but most other AMReX headers cannot and should be hidden by `#ifdef __cplusplus` if they are included. More details can be found at `amrex/Docs/Readme.typecheck`. Despite these limitations, it is recommended to use the type check tool and report issues to us.

Writing kernels in C++ is also an option. AMReX provides a multi-dimensional array type of syntax, similar to Fortran, that is readable and easy to implement. An example is given below:

```
void f (Box const& bx, FArrayBox& fab1, FArrayBox const& fab2)
{
    const auto len = length(bx);
    const auto lo = lbound(bx);
    const auto dst = fab1.view(lo);
    const auto src = fab2.view(lo);

    for (int k = 0; k < len.z; ++k) {
        for (int j = 0; j < len.y; ++j) {
            AMREX_PRAGMA SIMD
            for (int i = 0; i < len.x; ++i) {
                dst(i, j, k) = 0.5*(src(i, j, k)+src(i+1, j, k))
            }
        }
    }

    for (MFIter mfi(mf1,true); mfi.isValid(); ++mfi)
    {
        const Box& box = mfi.tilebox();
        f(box, mf1[mfi], mf2[mfi]);
    }
}
```

A `Box` and two `FArrayBoxes` are passed to a C++ kernel function. In the function, `amrex::length` is called to calculate and store the three-dimensional length of the loops based on the size of `bx`. `amrex::lbound` is called to get the lower bound of the `Box`. Both functions' return type is `amrex::Dim3`, a Plain Old Data type containing three integers. The result of `amrex::lbound` is then passed to `FArrayBox::view` to create a `FabView<FArrayBox>` that can be used to access the data.

`FabView<FArrayBox>` is an AMReX class that contains a pointer to the appropriate place in the global `FArrayBox` as well as an `operator()` that translates the three dimensional coordinates to the appropriate location in the one-dimensional array. It also translates between the global domain contained in the `FArrayBox` and the local work space defined by the `lo` array.

We put `AMREX_PRAGMA SIMD` macro above the innermost loop to notify the compiler that it is safe to vectorize the loop. This should be done whenever possible to achieve the best performance. The macro generates a compiler dependent pragma and their exact effect on the compiler is also compiler dependent. It should be emphasized that using the `AMREX_PRAGMA SIMD` macro on loops that are not safe for vectorization will lead to a variety of errors, so if unsure about the loop, test and verify before adding the macro.

Note that the view is shifted such that index 0 points to the lower end of the Box. To obtain the global index, the values needs to be shifted back using the appropriate `lo`. In the case of the example above, the global indices are: $(i+lo.x, j+lo.y, k+lo.z)$.

Also: be careful to use the appropriate `lo` array for each `FabView` object. If the loop works on two different global ranges, each `FabView` object must be created with the corresponding `lo` to obtain the correct data pointers.

4.17 Ghost Cells

AMReX uses a `MultiFab` as a container for floating point data on multiple Boxes at a single level of refinement. Each rectangular Box has its own boundaries on the low and high side in each coordinate direction. Each Box within a `MultiFab` can have ghost cells for storing data outside the Box's valid region. This allows us to, e.g., perform stencil-type operations on regular arrays. There are three basic types of boundaries:

1. interior boundary
2. coarse/fine boundary
3. physical boundary

Interior boundary is the border among the grid Boxes themselves. For example, in Fig. 4.1, the two blue grid Boxes on level 1 share an interior boundary that is 10 cells long. For a `MultiFab` with ghost cells on level 1, we can use the `MultiFab::FillBoundary` function introduced in the section on [FabArray, MultiFab and iMultiFab](#) to fill ghost cells at the interior boundary with valid cell data from other Boxes. `MultiFab::FillBoundary` can optionally fill periodic boundary ghost cells as well.

A coarse/fine boundary is the border between two AMR levels. `FillBoundary` does not fill these ghost cells. These ghost cells on the fine level need to be interpolated from the coarse level data. This is a subject that will be discussed in the section on [FillPatchUtil and Interpolator](#).

Note that periodic boundary is not considered a basic type in the discussion here because after periodic transformation it becomes either interior boundary or coarse/fine boundary.

The third type of boundary is the physical boundary at the physical domain. Note that both coarse and fine AMR levels could have grids touching the physical boundary. It is up to the application codes to properly fill the ghost cells at the physical boundary. However, AMReX does provide support for some common operations. See the section on [Boundary Conditions](#) for a discussion on domain boundary conditions in general, including how to implement physical (non-periodic) boundary conditions.

4.18 Boundary Conditions

This section describes how to implement domain boundary conditions in AMReX. A ghost cell that is outside of the valid region can be thought of as either “interior” (which includes periodic and coarse-fine ghost cells), or “physical”. Physical boundary conditions can occur on domain boundaries and can be characterized as inflow, outflow, slip/no-slip walls, etc., and are ultimately linked to mathematical Dirichlet or Neumann conditions.

The basic idea behind physical boundary conditions is as follows:

- Create a BCRec object, which is essentially a multidimensional integer array of $2 \times \text{DIM}$ components. Each component defines a boundary condition type for the lo/hi side of the domain, for each direction. See amrex/Src/Base/AMReX_BC_TYPES.H for common physical and mathematical types. If there is more than one variable, we can create an array of BCRec objects, and pass in a pointer to the 0-index component since the arrays for all the components are contiguous in memory. Here we need to provide boundary types to each component of the MultiFab. Below is an example of setting up `Vector<BCRec>` before the call to ghost cell routines.

```
// Set up BC; see ``amrex/Src/Base/AMReX_BC_TYPES.H`` for supported types
Vector<BCRec> bc(phi.nComp());
for (int n = 0; n < phi.nComp(); ++n)
{
    for (int idim = 0; idim < AMREX_SPACEDIM; ++idim)
    {
        if (Geometry::isPeriodic(idim))
        {
            bc[n].setLo(idim, BCType::int_dir); // interior
            bc[n].setHi(idim, BCType::int_dir);
        }
        else
        {
            bc[n].setLo(idim, BCType::foextrap); // first-order extrapolation
            bc[n].setHi(idim, BCType::foextrap);
        }
    }
}
```

`amrex::BCType` has the following types,

int_dir Interior, including periodic boundary

ext_dir “External Dirichlet”. It is the user’s responsibility to write a routine to fill ghost cells (more details below).

foextrap “First Order Extrapolation” First order extrapolation from last cell in interior.

reflect_even Reflection from interior cells with sign unchanged, $q(-i) = q(i)$.

reflect_odd Reflection from interior cells with sign changed, $q(-i) = -q(i)$.

- We have interfaces to a fortran routine that fills ghost cells at domain boundaries based on the boundary condition type defined in the BCRec object. It is the user’s responsibility to have a consistent definition of what the ghost cells represent. A common option used in AMReX codes is to fill the domain ghost cells with the value that lies on the boundary (as opposed to another common option where the value in the ghost cell represents an extrapolated value based on the boundary condition type). Then in our stencil based “work” codes, we also pass in the BCRec object and use modified stencils near the domain boundary that know the value in the first ghost cell represents the value on the boundary.

Depending on the level of complexity of your code, there are various options for filling domain boundary ghost cells.

For single-level codes built from amrex/Src/Base (excluding the amrex/Src/AmrCore and amrex/Src/Amr source code directories), you will have single-level MultiFabs filled with data in the valid region where you need to fill the ghost cells on each grid. There are essentially three ways to fill the ghost cells. (refer to amrex/Tutorials/Basic/HeatEquation_EX2_C for an example).

```
MultiFab mf;
Geometry geom;
Vector<BCRec> bc;
```

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```
// ...  
  
// fills interior and periodic domain boundary ghost cells  
mf.FillBoundary(geom.periodicity());  
  
// fills interior (but not periodic domain boundary) ghost cells  
mf.FillBoundary();  
  
// fills physical domain boundary ghost cells for a cell-centered multifab  
// except for external Dirichlet  
FillDomainBoundary(mf, geom, bc);
```

FillDomainBoundary() is a function in `amrex/Src/Base/AMReX_BCUtil.cpp` that fills the physical domain boundary ghost cells with Fortran function `amrex_fab_filcc` except for external Dirichlet (i.e., `BCType:ext_dir`). The user can use it as a template and insert their own function for `BCType:ext_dir` like below

```
if (! grown_domain_box.contains(fab_box))  
{  
    amrex_fab_filcc(BL_TO_FORTRAN_FAB(fab),  
                     BL_TO_FORTRAN_BOX(domain_box),  
                     dx, prob_lo,  
                     bc[0].data());  
    user_fab_filcc(BL_TO_FORTRAN_FAB(fab),  
                   BL_TO_FORTRAN_BOX(domain_box),  
                   dx, prob_lo,  
                   bc[0].data());  
}
```

4.19 Memory Allocation

AMReX has a Fortran module, `amrex_mempool_module` that can be used to allocate memory for Fortran pointers. The reason that such a module exists in AMReX, is that memory allocation is often very slow in multi-threaded OpenMP parallel regions. AMReX `amrex_mempool_module` provides a much faster alternative approach, in which each thread has its own memory pool. Here are examples of using the module.

```
use amrex_mempool_module, only : amrex_allocate, amrex_deallocate  
real(amrex_real), pointer, contiguous :: a(:,:,:,:), b(:,:,:,:)  
integer :: lo1, hi1, lo2, hi2, lo3, hi3, lo(4), hi(4)  
! lo1 = ...  
! a(lo1:hi1, lo2:hi2, lo3:hi3)  
call amrex_allocate(a, lo1, hi1, lo2, hi2, lo3, hi3)  
! b(lo(1):hi(1),lo(2):hi(2),lo(3):hi(3),lo(4):hi(4))  
call amrex_allocate(b, lo, hi)  
! .....  
call amrex_deallocate(a)  
call amrex_deallocate(b)
```

The downside of this is we have to use `pointer` instead of `allocatable`. This means we must explicitly free the memory via `amrex_deallocate` and we need to declare the pointers as `contiguous` for performance reason. Also, we often pass the Fortran pointer to a procedure with explicit array argument to get rid of the pointerness completely.

4.20 Abort, Assertion and Backtrace

`amrex::Abort(const char * message)` is used to terminate a run usually when something goes wrong. This function takes a message and writes it to stderr. Files named like `Backtrace.1` (where 1 means process 1) are produced containing backtrace information of the call stack. In Fortran, we can call `amrex_abort` from the `amrex_error_module`, which takes a Fortran character variable with assumed size (i.e., `len=*`) as a message. A `ParmParse` runtime boolean parameter `amrex.throw_handling` (which is defaulted to 0, i.e., `false`) can be set to 1 (i.e., `true`) so that AMReX will throw an exception instead of aborting.

`AMREX_ASSERT` is a macro that takes a Boolean expression. For debug build (e.g., `DEBUG=TRUE` using the GNU Make build system), if the expression at runtime is evaluated to false, `amrex::Abort` will be called and the run is thus terminated. For optimized build (e.g., `DEBUG=FALSE` using the GNU Make build system), the `AMREX_ASSERT` statement is removed at compile time and thus has no effect at runtime. We often use this as a means of putting debug statement in the code without adding any extra cost for production runs. For example,

```
AMREX_ASSERT(mf.nGrow() > 0 && mf.nComp() == mf2.nComp());
```

Here for debug build we like to assert that `MultiFab mf` has ghost cells and it also has the same number of components as `MultiFab mf2`. If we always want the assertion, we can use `AMREX_ALWAYS_ASSERT`. The assertion macros have a `_WITH_MESSAGE` variant that will print a message when assertion fails. For example,

```
AMREX_ASSERT_WITH_MESSAGE(mf.boxArray() == mf2.boxArray(),
                           "These two mfs must have the same BoxArray");
```

Backtrace files are produced by AMReX signal handler by default when segfault occurs or `Abort` is called. If the application does not want AMReX to handle this, `ParmParse` parameter `amrex.signal_handling=0` can be used to disable it.

4.21 Debugging

Debugging is an art. Everyone has their own favorite method. Here we offer a few tips we have found to be useful.

Compiling in debug mode (e.g., `make DEBUG=TRUE`) and running with `ParmParse` parameter `amrex.fpe_trap_invalid=1` can be helpful. In debug mode, many compiler debugging flags are turned on and all `MultiFab` data are initialized to signaling NaNs. The `amrex.fpe_trap_invalid` parameter will result in backtrace files when floating point exception occurs. One can then examine those files to track down the origin of the issue.

Writing a `MultiFab` to disk with

```
VisMF::Write(const FabArray<FArrayBox>& mf, const std::string& name)
```

in `AMReX_VisMF.H` and examining it with `Amrvis` (section [Amrvis](#)) can be helpful as well. In `AMReX_MultiFabUtil.H`, function

```
void print_state(const MultiFab& mf, const IntVect& cell, const int n=-1);
```

can output the data for a single cell.

Valgrind is one of our favorite debugging tool. For MPI runs, one can tell valgrind to output to different files for different processes. For example,

```
mpiexec -n 4 valgrind --leak-check=yes --track-origins=yes --log-file=vallog.%p ./foo.
↪exe ...
```

4.22 Example: HeatEquation_EX1_C

We now present an example of solving the heat equation. The source code tree for the heat equation example is simple, as shown in Fig. 4.3. We recommend you study `main.cpp` and `advance.cpp` to see some of the classes described below in action.

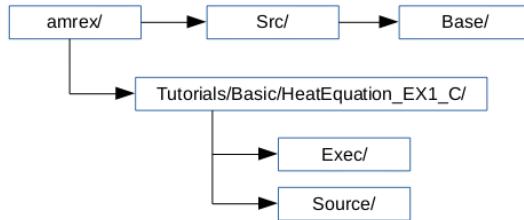


Fig. 4.3: Diagram of the source code structure for the HeatEquation_EX1_C example.

Source code tree for the HeatEquation_EX1_C example

amrex/Src/Base Contains source code for single-level simulations. Note that in `amrex/Src` there are many sub-directories, e.g., `Base`, `Amr`, `AmrCore`, `LinearSolvers`, etc. In this tutorial the only source code directory we need is `Base`.

amrex/Tutorials/HeatEquation_EX1_C/Source Contains the following source code specific to this tutorial:

1. `Make.package`: lists the source code files
2. `main.cpp`: contains the C++ main function
3. `advance.cpp`: advance the solution by a time step
4. `init_phi_Xd.f90`, `advance_Xd.f90`: fortran work functions used to initialize and advance the solution
5. `myfunc.H`: header file for C++ functions
6. `myfunc_F.H`: header file for fortran90 functions that are called in .cpp files

amrex/Tutorials/HeatEquation_EX1_C/Exec This is where you build the code with make. There is a GNUmakefile and inputs files, `inputs_2d` and `inputs_3d`.

Now we highlight a few key sections of the code. In `main.cpp` we demonstrate how to read in parameters from the inputs file:

```
// inputs parameters
{
    // ParmParse is way of reading inputs from the inputs file
    ParmParse pp;

    // We need to get n_cell from the inputs file - this is the number of cells on_
    ↪each side of
    // a square (or cubic) domain.
    pp.get("n_cell",n_cell);
```

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```
// The domain is broken into boxes of size max_grid_size
pp.get("max_grid_size",max_grid_size);

// Default plot_int to -1, allow us to set it to something else in the inputs file
// If plot_int < 0 then no plot files will be written
plot_int = -1;
pp.query("plot_int",plot_int);

// Default nsteps to 10, allow us to set it to something else in the inputs file
nsteps = 10;
pp.query("nsteps",nsteps);

pp.queryarr("is_periodic", is_periodic);
}
```

In main.cpp we demonstrate how to define a Box for the problem domain, and then how to chop that Box up into multiple boxes that define a BoxArray. We also define a Geometry object that knows about the problem domain, the physical coordinates of the box, and the periodicity:

```
// make BoxArray and Geometry
BoxArray ba;
Geometry geom;
{
    IntVect dom_lo(AMREX_D_DECL(      0,      0,      0));
    IntVect dom_hi(AMREX_D_DECL(n_cell-1, n_cell-1, n_cell-1));
    Box domain(dom_lo, dom_hi);

    // Initialize the boxarray "ba" from the single box "bx"
    ba.define(domain);
    // Break up boxarray "ba" into chunks no larger than "max_grid_size" along a_ ↵
    // direction
    ba.maxSize(max_grid_size);

    // This defines the physical box, [-1,1] in each direction.
    RealBox real_box({AMREX_D_DECL(-1.0,-1.0,-1.0)},
                      {AMREX_D_DECL( 1.0, 1.0, 1.0)});

    // This defines a Geometry object
    geom.define(domain,&real_box,CoordSys::cartesian,is_periodic.data());
}
```

In main.cpp we demonstrate how to build a DistributionMapping from the BoxArray, and then build MultiFabs with a desired number of components and ghost cells associated with each grid:

```
// Nghost = number of ghost cells for each array
int Nghost = 1;

// Ncomp = number of components for each array
int Ncomp = 1;

// How Boxes are distributed among MPI processes
DistributionMapping dm(ba);

// we allocate two phi multifabs; one will store the old state, the other the new.
MultiFab phi_old(ba, dm, Ncomp, Nghost);
MultiFab phi_new(ba, dm, Ncomp, Nghost);
```

We demonstrate how to build an array of face-based MultiFabs :

```
// build the flux multifabs
std::array<MultiFab, AMREX_SPACEDIM> flux;
for (int dir = 0; dir < AMREX_SPACEDIM; dir++)
{
    // flux(dir) has one component, zero ghost cells, and is nodal in direction dir
    BoxArray edge_ba = ba;
    edge_ba.surroundingNodes(dir);
    flux[dir].define(edge_ba, dm, 1, 0);
}
```

To access and/or modify data in a MultiFab we use the MFIter, where each processor loops over grids it owns to access and/or modify data on that grid:

```
// Initialize phi_new by calling a Fortran routine.
// MFIter = MultiFab Iterator
for ( MFIter mfi(phi_new); mfi.isValid(); ++mfi )
{
    const Box& bx = mfi.validbox();

    init_phi(BL_TO_FORTRAN_BOX(bx),
              BL_TO_FORTRAN_ANYD(phi_new[mfi]),
              geom.CellSize(), geom.ProbLo(), geom.ProbHi());
}
```

Note that these calls to fortran subroutines require a header in myfunc_F.H:

```
void init_phi(const int* lo, const int* hi,
               amrex_real* data, const int* dlo, const int* dhi,
               const amrex_real* dx, const amrex_real* prob_lo, const amrex_real* prob_hi);
```

The associated fortran routines must shape the data accordingly:

```
subroutine init_phi(lo, hi, phi, philo, phihi, dx, prob_lo, prob_hi) bind(C, name="init_phi")

use amrex_fort_module, only : amrex_real

implicit none

integer, intent(in) :: lo(2), hi(2), philo(2), phihi(2)
real(amrex_real), intent(inout) :: phi(philo(1):phihi(1),philo(2):phihi(2))
real(amrex_real), intent(in) :: dx(2)
real(amrex_real), intent(in) :: prob_lo(2)
real(amrex_real), intent(in) :: prob_hi(2)

integer :: i,j
double precision :: x,y,r2

do j = lo(2), hi(2)
    y = prob_lo(2) + (dble(j)+0.5d0) * dx(2)
    do i = lo(1), hi(1)
        x = prob_lo(1) + (dble(i)+0.5d0) * dx(1)
        r2 = ((x-0.25d0)**2 + (y-0.25d0)**2) / 0.01d0
    
```

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```
phi(i,j) = 1.d0 + exp(-r2)

end do
end do

end subroutine init_phi
```

Ghost cells are filled using the `FillBoundary` function:

```
// Fill the ghost cells of each grid from the other grids
// includes periodic domain boundaries
phi_old.FillBoundary(geom.periodicity());
```

CHAPTER

FIVE

TUTORIALS

AMReX Tutorials are a set of small stand-alone example codes that demonstrate how to use different parts of the AMReX functionality.

There is extensive documentation for the tutorial codes at https://amrex-codes.github.io/amrex/tutorials_html/

AMRCORE SOURCE CODE

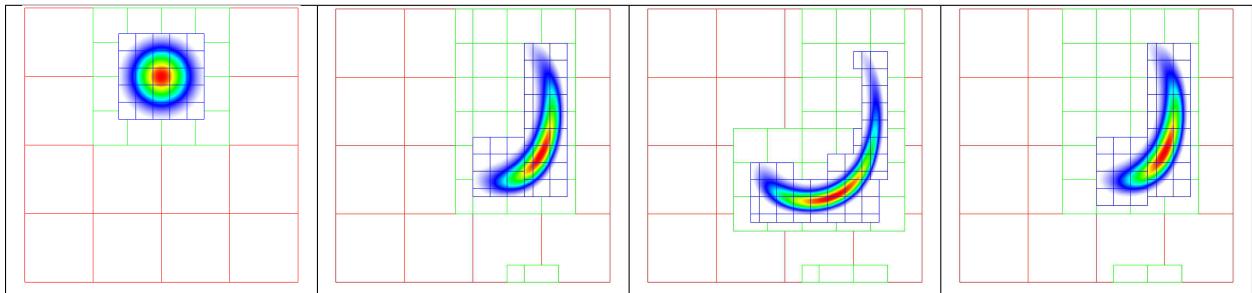
In this Chapter we give an overview of functionality contained in the `amrex/Src/AmrCore` source code. This directory contains source code for the following:

- Storing information about the grid layout and processor distribution mapping at each level of refinement.
- Functions to create grids at different levels of refinement, including tagging operations.
- Operations on data at different levels of refinement, such as interpolation and restriction operators.
- Flux registers used to store and manipulate fluxes at coarse-fine interfaces.
- Particle support for AMR (see [Particles](#)).

There is another source directory, `amrex/Src/Amr/`, which contains additional classes used to manage the time-stepping for AMR simulations. However, it is possible to build a fully adaptive, subcycling-in-time simulation code without these additional classes.

In this Chapter, we restrict our use to the `amrex/Src/AmrCore` source code and present a tutorial that performs an adaptive, subcycling-in-time simulation of the advection equation for a passively advected scalar. The accompanying tutorial code is available in `amrex/Tutorials/Amr/Advection_AmrCore` with build/run directory `Exec/SingleVortex`. In this example, the velocity field is a specified function of space and time, such that an initial Gaussian profile is displaced but returns to its original configuration at the final time. The boundary conditions are periodic and we use a refinement ratio of $r = 2$ between each AMR level. The results of the simulation in two-dimensions are depicted in the Table showing the [SingleVortex Tutorial](#).

Table 6.1: Time sequence ($t = 0, 0.5, 1, 1.5, 2$ s) of advection of a Gaussian profile using the `SingleVortex` tutorial. The red, green, and blue boxes indicate grids at AMR levels $\ell = 0, 1$, and 2 .



6.1 AmrCore Source Code: Details

Here we provide more information about the source code in `amrex/Src/AmrCore`.

6.1.1 AmrMesh and AmrCore

For single-level simulations (see e.g., `amrex/Tutorials/Basic/HeatEquation_EX1_C/main.cpp`) the user needs to build `Geometry`, `DistributionMapping`, and `BoxArray` objects associated with the simulation. For simulations with multiple levels of refinement, the `AmrMesh` class can be thought of as a container to store arrays of these objects (one for each level), and information about the current grid structure.

`amrex/Src/AmrCore/AMReX_AmrMesh.cpp/H` contains the `AmrMesh` class. The protected data members are:

```
protected:
    int          verbose;
    int          max_level;           // Maximum allowed level.
    Vector<IntVect> ref_ratio;     // Refinement ratios [0:finest_level-1]

    int          finest_level;       // Current finest level.

    Vector<IntVect> n_error_buf;    // Buffer cells around each tagged cell.
    Vector<IntVect> blocking_factor; // Blocking factor in grid generation
                                     // (by level).
    Vector<IntVect> max_grid_size;   // Maximum allowable grid size (by level).
    Real         grid_eff;           // Grid efficiency.
    int          n_proper;           // # cells required for proper nesting.

    bool         use_fixed_coarse_grids;
    int          use_fixed_upto_level;
    bool         refine_grid_layout; // chop up grids to have the number of
                                    // grids no less the number of procs

    Vector<Geometry>          geom;
    Vector<DistributionMapping> dmap;
    Vector<BoxArray>           grids;
```

The following parameters are frequently set via the inputs file or the command line. Their usage is described in the section on [Grid Creation](#)

Table 6.2: AmrCore parameters

| Variable | Value | Default |
|------------------------|-------|---------------------|
| amr.verbose | int | 0 |
| amr.max_level | int | none |
| amr.max_grid_size | ints | 32 in 3D, 128 in 2D |
| amr.n_proper | int | 1 |
| amr.grid_eff | Real | 0.7 |
| amr.n_error_buf | int | 1 |
| amr.blocking_factor | int | 8 |
| amr.refine_grid_layout | int | true |

`AMReX_AmrCore.cpp/H` contains the pure virtual class `AmrCore`, which is derived from the `AmrMesh` class. `AmrCore` does not actually have any data members, just additional member functions, some of which override the base class `AmrMesh`.

There are no pure virtual functions in `AmrMesh`, but there are 5 pure virtual functions in the `AmrCore` class. Any applications you create must implement these functions. The tutorial code `Amr/Advection_AmrCore` provides sample implementation in the derived class `AmrCoreAdv`.

```

///! Tag cells for refinement. TagBoxArray tags is built on level lev grids.
virtual void ErrorEst (int lev, TagBoxArray& tags, Real time,
                      int ngrow) override = 0;

///! Make a new level from scratch using provided BoxArray and DistributionMapping.
///! Only used during initialization.
virtual void MakeNewLevelFromScratch (int lev, Real time, const BoxArray& ba,
                                         const DistributionMapping& dm) override = 0;

///! Make a new level using provided BoxArray and DistributionMapping and fill
// with interpolated coarse level data.
virtual void MakeNewLevelFromCoarse (int lev, Real time, const BoxArray& ba,
                                         const DistributionMapping& dm) = 0;

///! Remake an existing level using provided BoxArray and DistributionMapping
// and fill with existing fine and coarse data.
virtual void RemakeLevel (int lev, Real time, const BoxArray& ba,
                           const DistributionMapping& dm) = 0;

///! Delete level data
virtual void ClearLevel (int lev) = 0;

```

Refer to the AmrCoreAdv class in the amrex/Tutorials/Amr/AmrCore_Advection/Source code for a sample implementation.

6.1.2 TagBox, and Cluster

These classes are used in the grid generation process. The TagBox class is essentially a data structure that marks which cells are “tagged” for refinement. Cluster (and ClusterList contained within the same file) are classes that help sort tagged cells and generate a grid structure that contains all the tagged cells. These classes and their member functions are largely hidden from any application codes through simple interfaces such as regrid and ErrorEst (a routine for tagging cells for refinement).

6.1.3 FillPatchUtil and Interpolator

Many codes, including the Advection_AmrCore example, contain an array of MultiFabs (one for each level of refinement), and then use “fillpatch” operations to fill temporary MultiFabs that may include a different number of ghost cells. Fillpatch operations fill all cells, valid and ghost, from actual valid data at that level, space-time interpolated data from the next-coarser level, neighboring grids at the same level, and domain boundary conditions (for examples that have non-periodic boundary conditions). Note that at the coarsest level, the interior and domain boundary (which can be periodic or prescribed based on physical considerations) need to be filled. At the non-coarsest level, the ghost cells can also be interior or domain, but can also be at coarse-fine interfaces away from the domain boundary. AMReX_FillPatchUtil.cpp/H contains two primary functions of interest.

1. FillPatchSingleLevel() fills a MultiFab and its ghost region at a single level of refinement. The routine is flexible enough to interpolate in time between two MultiFabs associated with different times.
2. FillPatchTwoLevels() fills a MultiFab and its ghost region at a single level of refinement, assuming there is an underlying coarse level. This routine is flexible enough to interpolate the coarser level in time first using FillPatchSingleLevel().

Note that FillPatchSingleLevel() and FillPatchTwoLevels() call the single-level routines MultiFab::FillBoundary and FillDomainBoundary() to fill interior, periodic, and physical boundary ghost cells. In principle, you can write a single-level application that calls FillPatchSingleLevel() instead of using MultiFab::FillBoundary and FillDomainBoundary().

A `FillPatchUtil` uses an `Interpolator`. This is largely hidden from application codes. `AMReX_Interpolater.cpp/H` contains the virtual base class `Interpolator`, which provides an interface for coarse-to-fine spatial interpolation operators. The `fillpatch` routines described above require an `Interpolator` for `FillPatchTwoLevels()`. Within `AMReX_Interpolater.cpp/H` are the derived classes:

- `NodeBilinear`
- `CellBilinear`
- `CellConservativeLinear`
- `CellConservativeProtected`
- `CellQuadratic`
- `PCInterp`
- `CellConservativeQuartic`

The Fortran routines that perform the actual work associated with `Interpolator` are contained in the files `AMReX_INTERP_F.H` and `AMReX_INTERP_xD.F`.

6.1.4 Using FluxRegisters

`AMReX_FluxRegister.cpp/H` contains the class `FluxRegister`, which is derived from the class `BndryRegister` (in `amrex/Src/Boundary/AMReX_BndryRegister`). In the most general terms, a `FluxRegister` is a special type of `BndryRegister` that stores and manipulates data (most often fluxes) at coarse-fine interfaces. A simple usage scenario comes from a conservative discretization of a hyperbolic system:

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \mathbf{F} \rightarrow \frac{\phi_{i,j}^{n+1} - \phi_{i,j}^n}{\Delta t} = \frac{F_{i+1/2,j} - F_{i-1/2,j}}{\Delta x} + \frac{F_{i,j+1/2} - F_{i,j-1/2}}{\Delta y}.$$

Consider a two-level, two-dimensional simulation. A standard methodology for advancing the solution in time is to first advance the coarse grid solution ignoring the fine level, and then advance the fine grid solution using the coarse level only to supply boundary conditions. At the coarse-fine interface, the area-weighted fluxes from the fine grid advance do not in general match the underlying flux from the coarse grid face, resulting in a lack of global conservation. Note that for subcycling-in-time algorithms (where for each coarse grid advance, the fine grid is advanced r times using a coarse grid time step reduced by a factor of r , where r is the refinement ratio), the coarse grid flux must be compared to the area *and* time-weighted fine grid fluxes. A `FluxRegister` accumulates and ultimately stores the net difference in fluxes between the coarse grid and fine grid advance over each face over a given coarse time step. The simplest possible synchronization step is to modify the coarse grid solution in coarse cells immediately adjacent to the coarse-fine interface are updated to account for the mismatch stored in the `FluxRegister`. This can be done “simply” by taking the coarse-level divergence of the data in the `FluxRegister` using the `reflux` function.

The Fortran routines that perform the actual floating point work associated with incrementing data in a `FluxRegister` are contained in the files `AMReX_FLUXREG_F.H` and `AMReX_FLUXREG_xD.F`.

6.1.5 AmrParticles and AmrParGDB

The `AmrCore/` directory contains derived classes for dealing with particles in a multi-level framework. The description of the base classes are given in the chapter on [Particles](#).

`AMReX_AmrParticles.cpp/H` contains the classes `AmrParticleContainer` and `AmrTracerParticleContainer`, which are derived from the classes `ParticleContainer` (in `amrex/Src/Particle/AMReX_Particles`) and `TracerParticleContainer` (in `amrex/Src/Particle/AMReX_TracerParticles`).

`AMReX_AmrParGDB.cpp/H` contains the class `AmrParGDB`, which is derived from the class `ParGDBBase` (in `amrex/Src/Particle/AMReX_ParGDB`).

6.2 Example: Advection_AmrCore

6.2.1 The Advection Equation

We seek to solve the advection equation on a multi-level, adaptive grid structure:

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot (\phi \mathbf{U}).$$

The velocity field is a specified divergence-free (so the flow field is incompressible) function of space and time. The initial scalar field is a Gaussian profile. To integrate these equations on a given level, we use a simple conservative update,

$$\frac{\phi_{i,j}^{n+1} - \phi_{i,j}^n}{\Delta t} = \frac{(\phi u)_{i+1/2,j}^{n+1/2} - (\phi u)_{i-1/2,j}^{n+1/2}}{\Delta x} + \frac{(\phi v)_{i,j+1/2}^{n+1/2} - (\phi v)_{i,j-1/2}^{n+1/2}}{\Delta y},$$

where the velocities on faces are prescribed functions of space and time, and the scalars on faces are computed using a Godunov advection integration scheme. The fluxes in this case are the face-centered, time-centered “ ϕu ” and “ ϕv ” terms.

We use a subcycling-in-time approach where finer levels are advanced with smaller time steps than coarser levels, and then synchronization is later performed between levels. More specifically, the multi-level procedure can most easily be thought of as a recursive algorithm in which, to advance level ℓ , $0 \leq \ell \leq \ell_{\max}$, the following steps are taken:

- Advance level ℓ in time by one time step, Δt^ℓ , as if it is the only level. If $\ell > 0$, obtain boundary data (i.e. fill the level ℓ ghost cells) using space- and time-interpolated data from the grids at $\ell - 1$ where appropriate.
- If $\ell < \ell_{\max}$
 - Advance level $(\ell + 1)$ for r time steps with $\Delta t^{\ell+1} = \frac{1}{r} \Delta t^\ell$.
 - Synchronize the data between levels ℓ and $\ell + 1$.



Fig. 6.1: Schematic of subcycling-in-time algorithm.

Specifically, for a 3-level simulation, depicted graphically in the figure showing the [Schematic of subcycling-in-time algorithm](#). above:

1. Integrate $\ell = 0$ over Δt .

2. Integrate $\ell = 1$ over $\Delta t/2$.
3. Integrate $\ell = 2$ over $\Delta t/4$.
4. Integrate $\ell = 2$ over $\Delta t/4$.
5. Synchronize levels $\ell = 1, 2$.
6. Integrate $\ell = 1$ over $\Delta t/2$.
7. Integrate $\ell = 2$ over $\Delta t/4$.
8. Integrate $\ell = 2$ over $\Delta t/4$.
9. Synchronize levels $\ell = 1, 2$.
10. Synchronize levels $\ell = 0, 1$.

For the scalar field, we keep track volume and time-weighted fluxes at coarse-fine interfaces. We accumulate area and time-weighted fluxes in `FluxRegister` objects, which can be thought of as special boundary FABsets associated with coarse-fine interfaces. Since the fluxes are area and time-weighted (and sign-weighted, depending on whether they come from the coarse or fine level), the flux registers essentially store the extent by which the solution does not maintain conservation. Conservation only happens if the sum of the (area and time-weighted) fine fluxes equals the coarse flux, which in general is not true.

The idea behind the level $\ell/(\ell+1)$ synchronization step is to correct for sources of mismatch in the composite solution:

1. The data at level ℓ that underlie the level $\ell+1$ data are not synchronized with the level $\ell+1$ data. This is simply corrected by overwriting covered coarse cells to be the average of the overlying fine cells.
2. The area and time-weighted fluxes from the level ℓ faces and the level $\ell+1$ faces do not agree at the $\ell/(\ell+1)$ interface, resulting in a loss of conservation. The remedy is to modify the solution in the coarse cells immediately next to the coarse-fine interface to account for the mismatch stored in the flux register (computed by taking the coarse-level divergence of the flux register data).

6.2.2 Code Structure



Fig. 6.2: Source code tree for the `AmrAdvection_AmrCore` example.

The figure shows the *Source code tree for the AmrAdvection_AmrCore example*.

- `amrex/Src/`
 - `Base/` Base amrex library.

- Boundary/ An assortment of classes for handling boundary data.
- AmrCore/ AMR data management classes, described in more detail above.
- Advection_AmrCore/Src Source code specific to this example. Most notably is the AmrCoreAdv class, which is derived from AmrCore. The subdirectories Src_2d and Src_3d contain dimension specific routines. Src_nd contains dimension-independent routines.
- Exec Contains a makefile so a user can write other examples besides SingleVortex.
- SingleVortex Build the code here by editing the GNUmakefile and running make. There is also problem-specific source code here used for initialization or specifying the velocity field used in this simulation.

Here is a high-level pseudo-code of the flow of the program:

```
/* Advection_AmrCore Pseudocode */
main()
    AmrCoreAdv amr_core_adv; // build an AmrCoreAdv object
    amr_core_adv.InitData() // initialize data all all levels
    AmrCore::InitFromScratch()
    AmrMesh::MakeNewGrids()
    AmrMesh::MakeBaseGrids() // define level 0 grids
    AmrCoreAdv::MakeNewLevelFromScratch()
    /* allocate phi_old, phi_new, t_new, and flux registers */
    initdata() // fill phi
    if (max_level > 0) {
        do {
            AmrMesh::MakeNewGrids()
            /* construct next finer grid based on tagging criteria */
            AmrCoreAdv::MakeNewLevelFromScratch()
            /* allocate phi_old, phi_new, t_new, and flux registers */
            initdata() // fill phi
        } (while (finest_level < max_level);
    }
    amr_core_adv.Evolve()
    loop over time steps {
        ComputeDt()
        timeStep() // advance a level
        /* check regrid conditions and regrid if necessary */
        Advance()
        /* copy phi into a MultiFab and fill ghost cells */
        /* advance phi */
        /* update flux registers */
        if (lev < finest_level) {
            timeStep() // recursive call to advance the next-finer level "r" times
            /* check regrid conditions and regrid if necessary */
            Advance()
            /* copy phi into a MultiFab and fill ghost cells */
            /* advance phi */
            /* update flux registers */
            reflux() // synchronize lev and lev+1 using FluxRegister divergence
            AverageDown() // set covered coarse cells to be the average of fine
        }
    }
}
```

6.2.3 The AmrCoreAdv Class

This example uses the class AmrCoreAdv, which is derived from the class AmrCore (which is derived from AmrMesh). The function definitions/implementations are given in AmrCoreAdv.H/cpp.

6.2.4 FluxRegisters

The function `AmrCoreAdv::Advance()` calls the Fortran subroutine, `advect` (in `./Src_xd/Adv_xd.f90`). `advect` computes and returns the time-advanced state as well as the fluxes used to update the state. These fluxes are used to set or increment the flux registers.

```
// increment or decrement the flux registers by area and time-weighted fluxes
// Note that the fluxes have already been scaled by dt and area
// In this example we are solving phi_t = -div(+F)
// The fluxes contain, e.g., F_{i+1/2,j} = (phi*u)_{i+1/2,j}
// Keep this in mind when considering the different sign convention for updating
// the flux registers from the coarse or fine grid perspective
// NOTE: the flux register associated with flux_reg[lev] is associated
// with the lev/lev-1 interface (and has grid spacing associated with lev-1)
if (do_reflux) {
    if (flux_reg[lev+1]) {
        for (int i = 0; i < BL_SPACEDIM; ++i) {
            flux_reg[lev+1]->CrseInit(fluxes[i], i, 0, 0, fluxes[i].nComp(), -1.0);
        }
    }
    if (flux_reg[lev]) {
        for (int i = 0; i < BL_SPACEDIM; ++i) {
            flux_reg[lev]->FineAdd(fluxes[i], i, 0, 0, fluxes[i].nComp(), 1.0);
        }
    }
}
```

The synchronization is performed at the end of `AmrCoreAdv::timeStep`:

```
if (do_reflux)
{
    // update lev based on coarse-fine flux mismatch
    flux_reg[lev+1]->Reflux(*phi_new[lev], 1.0, 0, 0, phi_new[lev]->nComp(),
                           geom[lev]);
}

AverageDownTo(lev); // average lev+1 down to lev
```

6.2.5 Regridding

The regrid function belongs to the `AmrCore` class (it is virtual – in this tutorial we use the instance in `AmrCore`).

At the beginning of each time step, we check whether we need to regrid. In this example, we use a `regrid_int` and keep track of how many times each level has been advanced. When any given particular level $\ell < \ell_{\max}$ has been advanced a multiple of `regrid_int`, we call the `regrid` function.

```
void
AmrCoreAdv::timeStep (int lev, Real time, int iteration)
{
    if (regrid_int > 0) // We may need to regrid
    {
        // regrid changes level "lev+1" so we don't regrid on max_level
        if (lev < max_level && istep[lev])
        {
            if (istep[lev] % regrid_int == 0)
            {

```

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```

    // regrid could add newly refine levels
    // (if finest_level < max_level)
    // so we save the previous finest level index
    int old_finest = finest_level;
    regrid(lev, time);

    // if there are newly created levels, set the time step
    for (int k = old_finest+1; k <= finest_level; ++k) {
        dt[k] = dt[k-1] / MaxRefRatio(k-1);
    }
}
}
}

```

Central to the regridding process is the concept of “tagging” which cells need refinement. ErrorEst is a pure virtual function of AmrCore, so each application code must contain an implementation. In AmrCoreAdv.cpp the ErrorEst function is essentially an interface to a Fortran routine that tags cells (in this case, state_error in Src_nd/Tagging_nd.f90). Note that this code uses tiling.

```

// tag all cells for refinement
// overrides the pure virtual function in AmrCore
void
AmrCoreAdv::ErrorEst (int lev, TagBoxArray& tags, Real time, int ngrow)
{
    static bool first = true;
    static Vector<Real> phierr;

    // only do this during the first call to ErrorEst
    if (first)
    {
        first = false;
        // read in an array of "phierr", which is the tagging threshold
        // in this example, we tag values of "phi" which are greater than phierr
        // for that particular level
        // in subroutine state_error, you could use more elaborate tagging, such
        // as more advanced logical expressions, or gradients, etc.
    ParmParse pp("adv");
    int n = pp.countval("phierr");
    if (n > 0) {
        pp.getarr("phierr", phierr, 0, n);
    }
}

if (lev >= phierr.size()) return;

const int clearval = TagBox::CLEAR;
const int tagval = TagBox::SET;

const Real* dx      = geom[lev].CellSize();
const Real* prob_lo = geom[lev].ProbLo();

const MultiFab& state = *phi_new[lev];

#ifndef _OPENMP
#pragma omp parallel
#endif

```

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```

{
    Vector<int> itags;

    for (MFIter mfi(state,true); mfi.isValid(); ++mfi)
    {
        const Box& tilebox = mfi.tilebox();

        TagBox& tagfab = tags[mfi];

        // We cannot pass tagfab to Fortran because it is BaseFab<char>.
        // So we are going to get a temporary integer array.
        // set itags initially to 'untagged' everywhere
        // we define itags over the tilebox region
        tagfab.get_itags(itags, tilebox);

        // data pointer and index space
        int* tptr = itags.dataPtr();
        const int* tlo = tilebox.loVect();
        const int* thi = tilebox.hiVect();

        // tag cells for refinement
        state_error(tptr, ARLIM_3D(tlo), ARLIM_3D(thi),
                    BL_TO_FORTRAN_3D(state[mfi]),
                    &tagval, &clearval,
                    ARLIM_3D(tilebox.loVect()), ARLIM_3D(tilebox.hiVect()),
                    ZFILL(dx), ZFILL(prob_lo), &time, &ph ierr[lev]);
        //
        // Now update the tags in the TagBox in the tilebox region
        // to be equal to itags
        //
        tagfab.tags_and_untags(itags, tilebox);
    }
}
}
}

```

The state_error subroutine in Src_nd/Tagging_nd.f90 in this example is simple:

```

subroutine state_error(tag,tag_lo,tag_hi, &
                      state,state_lo,state_hi, &
                      set,clear,&
                      lo,hi,&
                      dx,problo,time,ph ierr) bind(C, name="state_error")

implicit none

integer :: lo(3),hi(3)
integer :: state_lo(3),state_hi(3)
integer :: tag_lo(3),tag_hi(3)
double precision :: state(state_lo(1):state_hi(1), &
                           state_lo(2):state_hi(2), &
                           state_lo(3):state_hi(3))
integer :: tag(tag_lo(1):tag_hi(1), &
                tag_lo(2):tag_hi(2), &
                tag_lo(3):tag_hi(3))
double precision :: problo(3),dx(3),time,ph ierr
integer :: set,clear

```

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```

integer :: i, j, k

! Tag on regions of high phi
do      k = lo(3), hi(3)
  do      j = lo(2), hi(2)
    do i = lo(1), hi(1)
      if (state(i,j,k) .ge. ph ierr) then
        tag(i,j,k) = set
      endif
    enddo
  enddo
enddo

end subroutine state_error

```

6.2.6 Grid Creation

The gridding algorithm proceeds in this order, using the parameters described in the section on the [AmrCore Source Code: Details](#).

1. If at level 0, the domain is initially defined by `n_cell` as specified in the inputs file. If at level greater than 0, grids are created using the Berger-Rigoutsis clustering algorithm applied to the tagged cells from the section on [Regridding](#), modified to ensure that all new fine grids are divisible by `blocking_factor`.
2. Next, the grid list is chopped up if any grids are larger than `max_grid_size`. Note that because `max_grid_size` is a multiple of `blocking_factor` (as long as `max_grid_size` is greater than `blocking_factor`), the `blocking_factor` criterion is still satisfied.
3. Next, if `refine_grid_layout = 1` and there are more processors than grids at this level, then the grids at this level are further divided in order to ensure that no processor has less than one grid (at each level). In `AmrMesh::ChopGrids`,
 - if `max_grid_size / 2` in the `BL_SPACEDIM` direction is a multiple of `blocking_factor`, then chop the grids in the `BL_SPACEDIM` direction so that none of the grids are longer in that direction than `max_grid_size / 2`
 - If there are still fewer grids than processes, repeat the procedure in the `BL_SPACEDIM-1` direction, and again in the `BL_SPACEDIM-2` direction if necessary
 - If after completing a sweep in all coordinate directions with `max_grid_size / 2`, there are still fewer grids than processes, repeat the steps above with `max_grid_size / 4`.

6.2.7 FillPatch

This example has two functions, `AmrCoreAdv::FillPatch` and `AmrCoreAdv::CoarseFillPatch`, that make use of functions in `AmrCore/AMReX_FillPatchUtil`.

In `AmrCoreAdv::Advance`, we create a temporary `MultiFab` called `Sborder`, which is essentially ϕ but with ghost cells filled in. The valid and ghost cells are filled in from actual valid data at that level, space-time interpolated data from the next-coarser level, neighboring grids at the same level, or domain boundary conditions (for examples that have non-periodic boundary conditions).

```

MultiFab Sborder(grids[lev], dmap[lev], S_new.nComp(), num_grow);
FillPatch(lev, time, Sborder, 0, Sborder.nComp());

```

Several other calls to fillpatch routines are hidden from the user in the regridding process.

AMR SOURCE CODE

The source code in `amrex/Src/Amr` contains a number of classes, most notably `Amr`, `AmrLevel`, and `LevelBld`. These classes provide a more well developed set of tools for writing AMR codes than the classes created for the `Advection_AmrCore` tutorial.

- The `Amr` class is derived from `AmrCore`, and manages data across the entire AMR hierarchy of grids.
- The `AmrLevel` class is a pure virtual class for managing data at a single level of refinement.
- The `LevelBld` class is a pure virtual class for defining variable types and attributes.

Many of our mature, public application codes contain derived classes that inherit directly from `AmrLevel`. These include our compressible astrophysics code, CASTRO, (available in the AMReX-Astro/Castro github repository) and our computational cosmology code, Nyx (available in the AMReX-Astro/Nyx github repository). Our incompressible Navier-Stokes code, IAMR (available in the AMReX-codes/IAMR github repository) has a pure virtual class called `NavierStokesBase` that inherits from `AmrLevel`, and an additional derived class `NavierStokes`. Our low Mach number combustion code PeleLM (not yet public) also inherits from `NavierStokesBase`.

The tutorial code in `amrex/Tutorials/Amr/Advection_AmrLevel` gives a simple example of a class derived from `AmrLevel` that can be used to solve the advection equation on a subcycling-in-time AMR hierarchy. Note that example is essentially the same as the `amrex/Tutorials/Amr/Advection_AmrCore` tutorial and documentation in the chapter on [AmrCore Source Code](#), except now we use the provided libraries in `amrex/Src/Amr`.

The tutorial code also contains a `LevelBldAdv` class (derived from `LevelBld` in the `Source/Amr` directory). This class is used to define variable types (how many, nodality, interlevel interpolation stencils, etc.).

7.1 Amr Class

The `Amr` class is designed to manage parts of the computation which do not belong on a single level, like establishing and updating the hierarchy of levels, global timestepping, and managing the different `AmrLevels`. Most likely you will not need to derive any classes from `Amr`. Our mature application codes use this base class without any derived classes.

One of the most important data members is an array of `AmrLevels` - the `Amr` class calls many functions from the `AmrLevel` class to do things like advance the solution on a level, compute a time step to be used for a level, etc.

7.2 AmrLevel Class

Pure virtual functions include:

- `computeInitialDt` Compute an array of time steps for each level of refinement. Called at the beginning of the simulation.

- `computeNewDt` Compute an array of time steps for each level of refinement. Called at the end of a coarse level advance.
- `advance` Advance the grids at a level.
- `post_timestep` Work after at time step at a given level. In this tutorial we do the AMR synchronization here.
- `post_regrid` Work after regridding. In this tutorial we redistribute particles.
- `post_init` Work after initialization. In this tutorial we perform AMR synchronization.
- `initData` Initialize the data on a given level at the beginning of the simulation.
- `init` There are two versions of this function used to initialize data on a level during regridding. One version is specifically for the case where the level did not previously exist (a newly created refined level)
- `errorEst` Perform the tagging at a level for refinement.

7.2.1 StateData

The most important data managed by the `AmrLevel` is an array of `StateData`, which holds the scalar fields, etc., in the boxes that together make up the level.

`StateData` is a class that essentially holds a pair of `MultiFabs`: one at the old time and one at the new time. AMReX knows how to interpolate in time between these states to get data at any intermediate point in time. The main data that we care about in our applications codes (such as the fluid state) will be stored as `StateData`. Essentially, data is made `StateData` if we need it to be stored in checkpoints/plotfiles, and/or we want it to be automatically interpolated when we refine. An `AmrLevel` stores an array of `StateData` (in a C++ array called `state`). We index this array using integer keys (defined via an enum in, e.g., `AmrLevelAdv.H`):

```
enum StateType { Phi_Type = 0,
                 NUM_STATE_TYPE };
```

In our tutorial code, we use the function `AmrLevelAdv::variableSetup` to tell our simulation about the `StateData` (e.g., how many variables, ghost cells, nodality, etc.) Note that if you have more than one `StateType`, each of the different `StateData` carried in the state array can have different numbers of components, ghost cells, boundary conditions, etc. This is the main reason we separate all this data into separate `StateData` objects collected together in an indexable array.

7.3 LevelBld Class

The `LevelBld` class is a pure virtual class for defining variable types and attributes. To more easily understand its usage, refer to the derived class, `LevelBldAdv` in the tutorial. The `variableSetUp` and `variableCleanUp` are implemented, and in this tutorial call routines in the `AmrLevelAdv` class, e.g.,

```
void
AmrLevelAdv::variableSetUp ()
{
    BL_ASSERT(desc_lst.size() == 0);

    // Get options, set phys_bc
    read_params();

    desc_lst.addDescriptor(Phi_Type, IndexType::TheCellType(),
                          StateDescriptor::Point, 0, NUM_STATE,
```

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```

    &cell_cons_interp);

    int lo_bc[BL_SPACEDIM];
    int hi_bc[BL_SPACEDIM];
    for (int i = 0; i < BL_SPACEDIM; ++i) {
        lo_bc[i] = hi_bc[i] = INT_DIR;      // periodic boundaries
    }

    BCRec bc(lo_bc, hi_bc);

    desc_lst.setComponent(Phi_Type, 0, "phi", bc,
                          StateDescriptor::BndryFunc(nullfill));
}

```

We see how to define the `StateType`, including nodality, whether or not we want the variable to represent a point in time or an interval over time (useful for returning the time associated with data), the number of ghost cells, number of components, and the interlevel interpolation (See AMReX_Interpolator for various interpolation types). We also see how to specify physical boundary functions by providing a function (in this case, `nullfill` since we are not using physical boundary conditions), where `nullfill` is defined in a fortran routine in the tutorial source code.

7.4 Example: Advection_AmrLevel

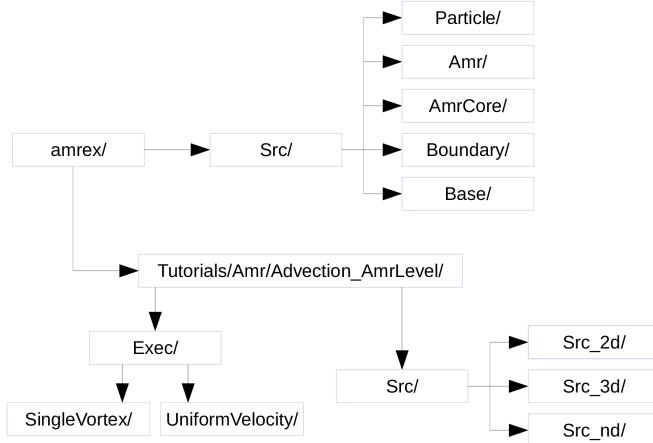


Fig. 7.1: Source code tree for the `AmrAdvection_AmrLevel` example.

The figure above shows the *Source code tree for the AmrAdvection_AmrLevel example*.

- amrex/Src/
 - Base/ Base amrex library.
 - Boundary/ An assortment of classes for handling boundary data.
 - AmrCore/ AMR data management classes, described in more detail above.
 - Amr/

- Advection_AmrLevel/Src Source code specific to this example. Most notably is the AmrLevelAdv class, which is derived from AmrLevel. The subdirectories Src_2d and Src_3d contain dimension specific routines. Src_nd contains dimension-independent routines.
- Exec Contains a makefile so a user can write other examples besides SingleVortex and UniformVelocity.
- SingleVortex and UniformVelocity Build the code here by editing the GNUmakefile and running make. There is also problem-specific source code here used for initialization or specifying the velocity field used in this simulation.

```
/* Advection_AmrLevel Pseudocode */
main()
{
    Amr amr;
    amr.init();
    loop {
        amr.coarseTimeStep();
        /* compute dt */
        timeStep();
        amr_level[level]->advance();
        /* call timeStep r times for next-finer level */
        amr_level[level]->post_timestep(); // AMR synchronization
        postCoarseTimeStep();
        /* write plotfile and checkpoint */
    }
    /* write final plotfile and checkpoint */
}
```

7.5 Particles

There is an option to turn on passively advected particles. In the GNUmakefile, add the line USE_PARTICLES = TRUE and build the code (do a make realclean first). In the inputs file, add the line adv.do_tracers = 1. When you run the code, within each plotfile directory there will be a subdirectory called “Tracer”.

Copy the files from amrex/Tools/Py_util/amrex_particles_to_vtp into the run directory and type, e.g.,

```
python amrex_binary_particles_to_vtp.py plt00000 Tracer
```

To generate a vtp file you can open with ParaView (Refer to the chapter on [Visualization](#)).

CHAPTER
EIGHT

ASYNCHRONOUS ITERATORS (AMRTASK)

Hiding communication overheads via overlapping communication with computation requires a sufficiently large amount of task parallelism. This problem is even more challenging due to various types of tasks in an AMReX program, including data parallel tasks (same workload on different data partitions) and control parallel tasks (different types of workload). This chapter introduces the API of AMReX's asynchronous iterators that can facilitate the job of identifying tasks in the applications. We have developed two iterators called FillPatch and RegionGraph Iterators, which will be described later on in this chapter. We first show how the programmer can use a runtime system to execute application codes written with these iterators.

In `amrex/Src/AmrTask/rts_impls`, we implement RTS - a runtime system that can execute asynchronous AMReX applications efficiently on large-scale systems. RTS is a black box to the application developer as showed in the following code snippet, which is the main function of a typical AMReX application running asynchronously under the control of the runtime system. The programmer first needs to use the namespace `perilla`, which covers all the C++ classes for the runtime system. To execute an AMR program (i.e. object of the `Amr` class), the programmer can simply create an object of RTS and pass the program object into the `Iterate` method. The runtime system will iteratively execute coarse time steps until the program completes. By default RTS links to MPI and Pthreads libraries. The programmer can also switch to other backends such as UPCXX (1-sided communication model compared to the common 2-sided model in MPI) without changing the application source code.

```
using namespace perilla;
int main (int argc, char* argv[])
{
    amrex::Initialize(argc,argv);
    ... //set up program input, e.g. start_time, stop_time, max_step
    Amr amr;
    amr.init(start_time,stop_time);
    RTS rts;
    rts.Iterate(&amr, max_step, stop_time);
    amrex::Finalize();
    return 0;
}
```

In a few functions of the `Amr` class, the runtime exposes multiple threads per process. As a result, the programmer needs to place sufficient memory protection for shared data within the process, e.g. when updating the state data. This multithreaded interface adds some programming cost, but is necessary for mitigating the task scheduling overhead. To avoid these programming details, the programmer can use built-in iterators, such as `fillpatch` iterator and task graph iterator that we next discuss. The API of these iterators is very simple, and the asynchronous code is very similar to the original code using the synchronous multifab iterator (`MFIter`) described earlier in chapter Basics.

8.1 FillPatch Iterator

FillPatch is an important operation commonly used in AMReX applications. This operation interpolates data in both space and time. Communication between AMR levels may incur when FillPatch interpolates data from a coarse AMR level and stores the result on the next finer level. This operation also results in communication within the same AMR level when the subcycling option is used, which requires data interpolation in time.

We develop an asynchronous version of the FillPatch operation, called Asynchronous FillPatch Iterator. Each iterator takes care of the communication with the previous and next subcycles at the same AMR level (time) and between the current and the next finer AMR levels (space and time). The iterator first automatically prepares temporary data needed for these communication activities and the data connections (aka data paths or data dependencies) among them.

Based on this setup, the programmer can design numerical solvers. This work is fairly simple. At a certain simulation time on an AMR level, the programmer can ask the runtime system which FABs have received sufficient data for advancing to the next time step. Although the FillPatch operation can be handled independently by the communication handler of the runtime system, this operation requires some computations such as packing/unpacking and extrapolation. The programmer has the freedom to dedicate a few threads from the pool of worker threads to parallelize those computations. This design choice may help the runtime process FillPatch operations faster, but may slow down the main computation. Thus, our advise to the programmer on using how many threads for the FillPatch is that it depends on the compute intensity of the actual workload. If the simulation is memory-bandwidth or network-bandwidth bound, the programmer can get the benefit from sparing more threads for doing FillPatch.

8.2 RegionGraph Iterator

We can simplify the programming work further with a new abstraction called RegionGraph Iterator a.k.a RGIter. This abstraction is a for loop (see the following code snippet), which can hide details of the asynchronous FillPatch Iterator in the init part and the graph traversal in the ++ operator. The only job required from the programmer is to specify the computations on the data, and they can easily place these computations in the loop body.

```
for (RGIter rgi(afpi_vec, upper_afpi_vec, ...); rgi.isValid(); ++rgi){  
    int f = rgi.currentRegion;  
    ...//computation on FAB f  
}
```

The execution of RGIter is as follows. Initially, an object of RGIter (i.e. rgi) is instantiated, taking vectors of FillPatch Iterators on the current and upper AMR levels as arguments (each element of the vector corresponds to a specific time). Based on these arguments, a task dependency graph spanning two AMR levels will be established. Next, isValid() asks the runtime system for FABs that have received all dependent data. When there is such a FAB, the computations in the loop body can execute on the FAB's data. When the computations on a FAB finish, the ++ operator is called. We overload this operator to traverse to the next runnable FAB.

Note: RGIter also supports data tiling. Specifically, we overload the ++ operator so that it will traverse data tiles in a FAB before it goes to next FAB if the tiling flag in the FAB is enabled. Instead of applying the computations in the loop body on the entire FAB, it executes them on a single tile at a time.

8.3 Generated Task Graph Code

The real input to the runtime system is an AMR program containing task dependency graphs (or task graph for short). Thus, the code written with the above asynchronous iterators will be transformed into a task graph form. The definition of a task dependency graph is as follows. Each task of a graph performs some computations on an FArrayBox (FAB). Tasks are connected with each other via edges, denoting the dependency on data. A task can be executed when all data dependencies have been satisfied. The code snippet below queries runnable tasks of a task dependency graph

named `regionGraph`. Note that each task dependency graph is more or less a wrapper of a `MultiFab`. In this example, a task of `regionGraph` computes the body code of the while loop to update the associated `FAB`. Each task of this graph receives data arrived at the runtime system and injects the data into the associated `FAB`. After updating `FAB`, it lets the runtime know about the change. The runtime system uses AMR domain knowledge to establish data dependencies among tasks, and thus it can answer which tasks are runnable and how to update neighbor `FABs` when a current `FAB` changes.

```
while (!regionGraph->isGraphEmpty())
{
    f = regionGraph->getAnyFireableRegion();
    multifabCopyPull(..., f, ...); //inject arrived dependent data into the fab, if any
    syncWorkerThreads();
    ...//compute on the fab f of multifab associated with coarseRegionGraph
    syncWorkerThreads();
    multifabCopyPush(..., f, ...); //tell the runtime that data of Fab f changed
    regionGraph->finalizeRegion(f)
}
```

The process of learning the domain knowledge is as follows. At the beginning of the program, the runtime extracts the metadata needed for establishing data dependencies among tasks of the same graph or between two different graphs. Every time the AMR grid hierarchy changes (i.e. when a few or all AMR levels regrid), the runtime re-extracts the metadata to correct the task dependency graphs. Once the metadata extraction completes, the runtime system invokes the computation on AMR levels (e.g., `timeStep`, `initTimeStep`, and `postTimeStep`).

I/O (PLOTFILE, CHECKPOINT)

In this chapter, we will discuss parallel I/O capabilities for mesh data in AMReX. The section on [Particle IO](#) will discuss I/O for particle data.

9.1 Plotfile

AMReX has its own native plotfile format. Many visualization tools are available for AMReX plotfiles (see the chapter on [Visualization](#)). AMReX provides the following two functions for writing a generic AMReX plotfile. Many AMReX application codes may have their own plotfile routines that store additional information such as compiler options, git hashes of the source codes and ParmParse runtime parameters.

```
void WriteSingleLevelPlotfile (const std::string &plotfilename,
                               const MultiFab &mf,
                               const Vector<std::string> &varnames,
                               const Geometry &geom,
                               Real time,
                               int level_step);

void WriteMultiLevelPlotfile (const std::string &plotfilename,
                             int nlevels,
                             const Vector<const MultiFab*> &mf,
                             const Vector<std::string> &varnames,
                             const Vector<Geometry> &geom,
                             Real time,
                             const Vector<int> &level_steps,
                             const Vector<IntVect> &ref_ratio);
```

`WriteSingleLevelPlotfile` is for single level runs and `WriteMultiLevelPlotfile` is for multiple levels. The name of the plotfile is specified by the `plotfilename` argument. This is the top level directory name for the plotfile. In AMReX convention, the plotfile name consist of letters followed by numbers (e.g., `plt00258`). `amrex::Concatenate` is a useful helper function for making such strings.

```
int istep = 258;
const std::string& pfname = amrex::Concatenate("plt",istep); // plt00258

// By default there are 5 digits, but we can change it to say 4.
const std::string& pfname2 = amrex::Concatenate("plt",istep,4); // plt0258

istep =1234567; // Having more than 5 digits is OK.
const std::string& pfname3 = amrex::Concatenate("plt",istep); // plt12344567
```

The argument `mf` above (`MultiFab` for single level and `Vector<const MultiFab*>` for multi-level) is the data to be written to the disk. Note that many visualization tools expect this to be cell-centered data. So for nodal

data, we need to convert them to cell-centered data through some kind of averaging. Also note that if you have data at each AMR level in several MultiFab, you need to build a new MultiFab at each level to hold all the data on that level. This involves local data copy in memory and is not expected to significantly increase the total wall time for writing plotfiles. For the multi-level version, the function expects `Vector<const MultiFab*>`, whereas the multi-level data are often stored as `Vector<std::unique_ptr<MultiFab>>`. AMReX has a helper function for this and one can use it as follows,

```
WriteMultiLevelPlotfile(....., amrex::GetVecOfConstPtrs(mf), ....);
```

The argument `varnames` has the names for each component of the MultiFab data. The size of the Vector should be equal to the number of components. The argument `geom` is for passing `Geometry` objects that contain the physical domain information. The argument `time` is for the time associated with the data. The argument `level_step` is for the current time step associated with the data. For multi-level plotfiles, the argument `nlevels` is the total number of levels, and we also need to provide the refinement ratio via an `Vector` of size `nlevels-1`.

We note that AMReX does not overwrite old plotfiles if the new plotfile has the same name. The old plotfiles will be renamed to new directories named like `plt00350.old.46576787980`.

9.2 Checkpoint File

Checkpoint files are used for restarting simulations from where the checkpoints are written. Each application code has its own set of data needed for restart. AMReX provides I/O functions for basic data structures like `MultiFab` and `BoxArray`. These functions can be used to build codes for reading and writing checkpoint files. Since each application code has its own requirement, there is no standard AMReX checkpoint format. However we have provided an example restart capability in the tutorial `/amrex/Tutorials/Amr/Advection_AmrCore/Exec/SingleVortex`. Refer to the functions `ReadCheckpointFile()` and `WriteCheckpointFile()` in this tutorial.

A checkpoint file is actually a directory with name, e.g., `chk00010` containing a `Header` (text) file, along with subdirectories `Level_0`, `Level_1`, etc. containing the `MultiFab` data at each level of refinement. The `Header` file contains problem-specific data (such as the finest level, simulation time, time step, etc.), along with a printout of the `BoxArray` at each level of refinement.

When starting a simulation from a checkpoint file, a typical sequence in the code could be:

- Read in the `Header` file data (except for the `BoxArray` data).
- For each level of refinement, do the following in order:
 - Read in the `BoxArray`
 - Build a `DistributionMapping`
 - Define any `MultiFab`, `FluxRegister`, etc. objects that are built upon the `BoxArray` and the `DistributionMapping`
 - Read in the `MultiFab` data

We do this one level at a time because when you create a distribution map, it checks how much allocated `MultiFab` data already exists before assigning grids to processors.

Typically a checkpoint file is a directory containing some text files and sub-directories (e.g., `Level_0` and `Level_1`) containing various data. It is a good idea that we first make these directories ready for subsequently writing to the disk. For example, to build directories `chk00010`, `chk00010/Level_0`, and `chk00010/Level_1`, you could write:

```
const std::string& checkpointname = amrex::Concatenate("chk", 10);  
  
amrex::Print() << "Writing checkpoint " << checkpointname << "\n";
```

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```

const int nlevels = 2;

bool callBarrier = true;

// ---- prebuild a hierarchy of directories
// ---- dirName is built first. if dirName exists, it is renamed. then build
// ---- dirName/subDirPrefix_0 .. dirName/subDirPrefix_nlevels-1
// ---- if callBarrier is true, call ParallelDescriptor::Barrier()
// ---- after all directories are built
// ---- ParallelDescriptor::IOProcessor() creates the directories
amrex::PreBuildDirectorHierarchy(checkpointname, "Level_", nlevels, callBarrier);

```

A checkpoint file of AMReX application codes often has a clear text Header file that only the I/O process writes to it using `std::ofstream`. The Header file contains problem-dependent information such as the time, the physical domain size, grids, etc. that are necessary for restarting the simulation. To guarantee that precision is not lost for storing floating point number like time in clear text file, the file stream's precision needs to be set properly. And a stream buffer can also be used. For example,

```

// write Header file
if (ParallelDescriptor::IOProcessor()) {

    VisMF::IO_Buffer io_buffer(VisMF::IO_Buffer_Size);
    std::ofstream HeaderFile;
    HeaderFile.rdbuf()->pubsetbuf(io_buffer.dataPtr(), io_buffer.size());
    std::string HeaderFileName(checkpointname + "/Header");
    HeaderFile.open(HeaderFileName.c_str(), std::ofstream::out | 
                    std::ofstream::trunc | 
                    std::ofstream::binary);

    if( ! HeaderFile.good()) {
        amrex::FileOpenFailed(HeaderFileName);
    }

    HeaderFile.precision(17);

    // write out title line
    HeaderFile << "Checkpoint file for AmrCoreAdv\n";

    // write out finest_level
    HeaderFile << finest_level << "\n";

    // write out array of istep
    for (int i = 0; i < istep.size(); ++i) {
        HeaderFile << istep[i] << " ";
    }
    HeaderFile << "\n";

    // write out array of dt
    for (int i = 0; i < dt.size(); ++i) {
        HeaderFile << dt[i] << " ";
    }
    HeaderFile << "\n";

    // write out array of t_new
    for (int i = 0; i < t_new.size(); ++i) {

```

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```

        HeaderFile << t_new[i] << " ";
    }
    HeaderFile << "\n";

    // write the BoxArray at each level
    for (int lev = 0; lev <= finest_level; ++lev) {
        boxArray(lev).writeOn(HeaderFile);
        HeaderFile << '\n';
    }
}

```

`amrex::VisMF` is a class that can be used to perform `MultiFab` I/O in parallel. How many processes are allowed to perform I/O simultaneously can be set via

```
VisMF::SetNOutFiles(64); // up to 64 processes, which is also the default.
```

The optimal number is of course system dependent. The following code shows how to write a `MultiFab`.

```

// write the MultiFab data to, e.g., chk00010/Level_0/
for (int lev = 0; lev <= finest_level; ++lev) {
    VisMF::Write(phi_new[lev],
                 amrex::MultiFabFileFullPrefix(lev, checkpointname, "Level_", "phi"));
}

```

It should also be noted that all the data including those in ghost cells are written/read by `VisMF::Write/Read`.

For reading the Header file, AMReX can have the I/O process read the file from the disk and broadcast it to others as `Vector<char>`. Then all processes can read the information with `std::istringstream`. For example,

```

std::string File(restart_chkfile + "/Header");

VisMF::IO_Buffer io_buffer(VisMF::GetIOBufferSize());

Vector<char> fileCharPtr;
ParallelDescriptor::ReadAndBcastFile(File, fileCharPtr);
std::string fileCharPtrString(fileCharPtr.dataPtr());
std::istringstream is(fileCharPtrString, std::istringstream::in);

std::string line, word;

// read in title line
std::getline(is, line);

// read in finest_level
is >> finest_level;
GotoNextLine(is);

// read in array of istep
std::getline(is, line);
{
    std::istringstream lis(line);
    int i = 0;
    while (lis >> word) {
        istep[i++] = std::stoi(word);
    }
}

```

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```
// read in array of dt
std::getline(is, line);
{
    std::istringstream lis(line);
    int i = 0;
    while (lis >> word) {
        dt[i++] = std::stod(word);
    }
}

// read in array of t_new
std::getline(is, line);
{
    std::istringstream lis(line);
    int i = 0;
    while (lis >> word) {
        t_new[i++] = std::stod(word);
    }
}
```

The following code how to read in a BoxArray, create a DistributionMapping, build MultiFab and FluxRegister data, and read in a MultiFab from a checkpoint file, on a level-by-level basis:

```
for (int lev = 0; lev <= finest_level; ++lev) {

    // read in level 'lev' BoxArray from Header
    BoxArray ba;
    ba.readFrom(is);
    GotoNextLine(is);

    // create a distribution mapping
    DistributionMapping dm { ba, ParallelDescriptor::NProcs() };

    // set BoxArray grids and DistributionMapping dmap in AMReX_AmrMesh.H class
    SetBoxArray(lev, ba);
    SetDistributionMap(lev, dm);

    // build MultiFab and FluxRegister data
    int ncomp = 1;
    int nghost = 0;
    phi_old[lev].define(grids[lev], dmap[lev], ncomp, nghost);
    phi_new[lev].define(grids[lev], dmap[lev], ncomp, nghost);
    if (lev > 0 && do_reflux) {
        flux_reg[lev].reset(new FluxRegister(grids[lev], dmap[lev], refRatio(lev-1),
                                         lev, ncomp));
    }
}

// read in the MultiFab data
for (int lev = 0; lev <= finest_level; ++lev) {
    VisMF::Read(phi_new[lev],
                 amrex::MultiFabFileFullPrefix(lev, restart_chkfile, "Level_", "phi"));
}
```

It should be emphasized that calling `VisMF::Read` with an empty MultiFab (i.e., no memory allocated for floating point data) will result in a MultiFab with a new `DistributionMapping` that could be different from any other existing `DistributionMapping` objects and is not recommended.

LINEAR SOLVERS

In this Chapter we give an overview of the linear solvers in AMReX that solve linear systems in the canonical form

$$(\alpha A - \beta \nabla \cdot B \nabla) \phi = f, \quad (10.1)$$

where α and β are scalar constants, A and B are scalar fields, ϕ is the unknown, and f is the right-hand side of the equation. Note that Poisson's equation $\nabla^2 \phi = f$ is a special case the canonical form. The sought solution ϕ is at either cell centers or nodes. For the cell-centered solver, A , ϕ and f are represented by cell-centered MultiFab, and B is represented by AMREX_SPACEDIM face type MultiFab. That is there are 1, 2 and 3 MultiFab representing B for 1, 2 and 3D, respectively. For the nodal solver, A is assumed to be zero, ϕ and f are nodal, and B is cell-centered. AMReX supports both single-level solve and composite solve on multiple AMR levels.

The tutorials in `amrex/Tutorials/LinearSolvers/` show examples of using the solvers. The tutorial `amrex/Tutorials/Basic/HeatEquation_EX3_C` shows how to solve the heat equation implicitly using the solver. The tutorials also show how to add linear solvers into the build system.

10.1 MLMG and Linear Operator Classes

MLMG is a class for solving the linear system using the geometric multigrid method. The constructor of MLMG takes the reference to MLLinOp, an abstract base class of various linear operator classes, MLABecLaplacian, MLPoisson, MLNodeLaplacian, etc. We choose the type of linear operator class according to the type the linear system to solve.

- MLABecLaplacian for cell-centered canonical form (equation (10.1)).
- MLPoisson for cell-centered constant coefficient Poisson's equation $\nabla^2 \phi = f$.
- MLNodeLaplacian for nodal variable coefficient Poisson's equation $\nabla \cdot (\sigma \nabla \phi) = f$.

The constructors of these linear operator classes are in the form like below

```
MLABecLaplacian (const Vector<Geometry>& a_geom,
                  const Vector<BoxArray>& a_grids,
                  const Vector<DistributionMapping>& a_dmap,
                  const LPInfo& a_info = LPInfo(),
                  const Vector<FabFactory<FArrayBox> const*>& a_factory = {});
```

It takes Vectors of Geometry, BoxArray and DistributionMapping. The arguments are Vectors because MLMG can do multi-level composite solve. If you are using it for single-level, you can do

```
// Given Geometry geom, BoxArray grids, and DistributionMapping dmap on single level
MLABecLaplacian mlabeclap({geom}, {grids}, {dmap});
```

to let the compiler construct `Vectors` for you. Recall that the classes `Vector`, `Geometry`, `BoxArray`, and `DistributionMapping` are defined in chapter [Basics](#). There are two new classes that are optional parameters. `LPInfo` is a class for passing parameters. `FabFactory` is used in problems with embedded boundaries (chapter [Embedded Boundaries](#)).

After the linear operator is built, we need to set up boundary conditions. This will be discussed later in section [Boundary Conditions](#).

For `MLABeLaplacian`, we next need to call member functions

```
void setScalars (Real alpha, Real beta);
void setACoeffs (int amrlev, const MultiFab& A);
void setBCoeffs (int amrlev, const Array<MultiFab const*>, AMREX_SPACEDIM>& B);
```

to set up the coefficients for equation (10.1). This is unnecessary for `MLPoisson`, as there are no coefficients to set. For `MLNodeLaplacian`, one needs to call the member function

```
void setSigma (int amrlev, const MultiFab& a_sigma);
```

The `int amrlev` parameter should be zero for single-level solves. For multi-level solves, each level needs to be provided with `A` and `B`, or `Sigma`. For composite solves, `amrlev 0` will mean the lowest level for the solver, which is not necessarily the lowest level in the AMR hierarchy. This is so solves can be done on different sections of the AMR hierarchy, e.g. on AMR levels 3 to 5.

After boundary conditions and coefficients are prescribed, the linear operator is ready for an `MLMG` object like below.

```
MLMG mlmg (mlabeclaplacian);
```

Optional parameters can be set (see section [Parameters](#)), and then we can use the `MLMG` member function

```
Real solve (const Vector<MultiFab*>& a_sol,
            const Vector<MultiFab const*>& a_rhs,
            Real a_tol_rel, Real a_tol_abs);
```

to solve the problem given an initial guess and a right-hand side. Zero is a perfectly fine initial guess. The two `Reals` in the argument list are the targeted relative and absolute error tolerances. The solver will terminate when one of these targets is met. Set the absolute tolerance to zero if one does not have a good value for it. The return value of `solve` is the max-norm error.

After the solver returns successfully, if needed, we can call

```
void compResidual (const Vector<MultiFab*>& a_res,
                    const Vector<MultiFab*>& a_sol,
                    const Vector<MultiFab const*>& a_rhs);
```

to compute residual (i.e., $f - L(\phi)$) given the solution and the right-hand side. For cell-centered solvers, we can also call the following functions to compute gradient $\nabla\phi$ and fluxes $-B\nabla\phi$.

```
void getGradSolution (const Vector<Array<MultiFab*, AMREX_SPACEDIM> >& a_grad_sol);
void getFluxes      (const Vector<Array<MultiFab*, AMREX_SPACEDIM> >& a_fluxes);
```

10.2 Boundary Conditions

We now discuss how to set up boundary conditions for linear operators. In the following, physical domain boundaries refer to the boundaries of the physical domain, whereas coarse/fine boundaries refer to the boundaries between AMR levels. The following steps must be followed in the exact order.

First we need to set physical domain boundary types via `MLLinOp` member function

```
void setDomainBC (const Array<BCType, AMREX_SPACEDIM>& ldbc, // for lower ends
const Array<BCType, AMREX_SPACEDIM>& hdbc); // for higher ends
```

The supported BC types at the physical domain boundaries are

- `LinOpBCType::Periodic` for periodic boundary.
- `LinOpBCType::Dirichlet` for Dirichlet boundary condition.
- `LinOpBCType::Neumann` for homogeneous Neumann boundary condition.
- `LinOpBCType::reflect_odd` for reflection with sign changed.

The second step is to set up coarse/fine Dirichlet boundary conditions. This step is not always needed. But when it is, it must be completed before step 3. This step is not needed when the coarsest level in the solver covers the whole computational domain (e.g., the coarsest level is AMR level 0). Note that this step is still needed in the case that the solver is used to do a single-level solve on a fine AMR level not covering the whole domain. The `MLLinOp` member function for this step is

```
void setCoarseFineBC (const MultiFab* crse, int crse_ratio);
```

Here `const MultiFab* crse` contains the Dirichlet boundary values at the coarse resolution, and `int crse_ratio` (e.g., 2) is the refinement ratio between the coarsest solver level and the AMR level below it.

In the third step, for each level, we call `MLLinOp` member function

```
virtual void setLevelBC (int amrlev, const MultiFab* levelbcdat) = 0;
```

to set up Dirichlet boundary values. Here the `MultiFab` must have one ghost cell. Although `MultiFab` is used to pass the data, only the values in the ghost cells at Dirichlet boundaries are used. If there are no Dirichlet boundaries, we still need to make this call, but we could call it with `nullptr`. It should be emphasized that the data in `levelbcdat` for Dirichlet boundaries are assumed to be exactly on the face of the physical domain even though for cell-centered solvers the sought unknowns are at cell centers. And for cell-centered solvers, the `MultiFab` argument must have the cell-centered type.

10.3 Parameters

There are many parameters that can be set. Here we discuss some commonly used ones.

`MLLinOp::setVerbose(int)`, `MLMG::setVerbose(int)` and `MLMG::setBottomVerbose(int)` can be control the verbosity of the linear operator, multigrid solver and the bottom solver, respectively.

The multigrid solver is an iterative solver. The maximal number of iterations can be changed with `MLMG::setMaxIter(int)`. We can also do a fixed number of iterations with `MLMG::setFixedIter(int)`. By default, V-cycle is used. We can use `MLMG::setMaxFmgIter(int)` to control how many full multigrid cycles can be done before switching to V-cycle.

`LPInfo::setMaxCoarseningLevel(int)` can be used to control the maximal number of multigrid levels. We usually should not call this function. However, we sometimes build the solver to simply apply the operator (e.g., $L(\phi)$) without needing to solve the system. We can do something as follows to avoid the cost of building coarsened operators for the multigrid.

```
MLABecLaplacian mlabeclap({geom}, {grids}, {dmap}, LPInfo().setMaxCoarseningLevel(0));
// set up BC
// set up coefficients
```

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```
MLMG mlmg(mlabeclap);
// out = L(in)
mlmg.apply(out, in); // here both in and out are const Vector<MultiFab*>&
```

At the bottom of the multigrid cycles, we use the biconjugate gradient stabilized method as the bottom solver. MLMG member method

```
void setBottomSolver (BottomSolver s);
```

can be used to change the bottom solver. Available choices are

- MLMG::BottomSolver::smoother: Smoother such as Gauss-Seidel.
- MLMG::BottomSolver::bicgstab: The default.
- MLMG::BottomSolver::cg: The conjugate gradient method. The matrix must be symmetric.
- MLMG::BottomSolver::Hypre: BoomerAMG in HYPRE. Currently for cell-centered only.

10.4 Curvilinear Coordinates

The linear solvers support curvilinear coordinates including 1D spherical and 2d cylindrical (r, z). In those cases, the divergence operator has extra metric terms. If one does not want the solver to include the metric terms because they have been handled in other ways, one can call `setMetricTerm(bool)` with `false` on the `LPIInfo` object passed to the constructor of linear operators.

10.5 HYPRE

AMReX can use HYPRE BoomerAMG as a bottom solver (currently for cell-centered problems only), as we have mentioned. For challenging problems, our geometric multigrid solver may have difficulty solving, whereas an algebraic multigrid method might be more robust. We note that by default our solver always tries to geometrically coarsen the problem as much as possible. However, as we have mentioned, we can call `setMaxCoarseningLevel(0)` on the `LPIInfo` object passed to the constructor of a linear operator to disable the coarsening completely. In that case the bottom solver is solving the residual correction form of the original problem. To use HYPRE, one must include `amrex/Src/Extern/HYPRE` in the build system. For an example of using HYPRE, we refer the reader to `Tutorials/LinearSolvers/ABecLaplacian_C`.

10.6 Embedded Boundaries

AMReX support solving linear systems with embedded boundaries. See chapter *Embedded Boundaries* for more details.

PARTICLES

In addition to the tools for working with mesh data described in previous chapters, AMReX also provides data structures and iterators for performing data-parallel particle simulations. Our approach is particularly suited to particles that interact with data defined on a (possibly adaptive) block-structured hierarchy of meshes. Example applications include Particle-in-Cell (PIC) simulations, Lagrangian tracers, or particles that exert drag forces onto a fluid, such as in multi-phase flow calculations. The overall goals of AMReX's particle tools are to allow users flexibility in specifying how the particle data is laid out in memory and to handle the parallel communication of particle data. In the following sections, we give an overview of AMReX's particle classes and how to use them.

11.1 The Particle

The particle classes can be used by including the header `AMReX_Particles.H`. The most basic particle data structure is the particle itself:

```
Particle<3, 2> p;
```

This is a templated data type, designed to allow flexibility in the number and type of components that the particles carry. The first template parameter is the number of extra `Real` variables this particle will have (either single or double precision¹), while the second is the number of extra integer variables. It is important to note that this is the number of *extra* real and integer variables; a particle will always have at least `BL_SPACEDIM` real components that store the particle's position and 2 integer components that store the particle's `id` and `cpu` numbers.²

The particle struct is designed to store these variables in a way that minimizes padding, which in practice means that the `Real` components always come first, and the integer components second. Additionally, the required particle variables are stored before the optional ones, for both the real and the integer components. For example, say we want to define a particle type that stores a mass, three velocity components, and two extra integer flags. Our particle struct would be set up like:

```
Particle<4, 2> p;
```

and the order of the particle components in would be (assuming `BL_SPACEDIM` is 3): `x y z m vx vy vz id`
`cpu flag1 flag2`.³

¹ Particles default to double precision for their real data. To use single precision, compile your code with `USE_SINGLE_PRECISION_PARTICLES=TRUE`.

² Note that `cpu` stores the number of the process the particle was *generated* on, not the one it's currently assigned to. This number is set on initialization and never changes, just like the particle `id`. In essence, the particles have two integer `id` numbers, and only the combination of the two is unique. This was done to facilitate the creation of particle initial conditions in parallel.

³ Note that for the extra particle components, which component refers to which variable is an application-specific convention - the particles have 4 extra real comps, but which one is "mass" is up to the user. We suggest using an `enum` to keep these indices straight; please see `amrex/Tutorials/Particles/ElectrostaticPIC/ElectrostaticParticleContainer.H` for an example of this.

11.1.1 Setting Particle data

The `Particle` struct provides a number of methods for getting and setting a particle's data. For the required particle components, there are special, named methods. For the “extra” real and integer data, you can use the `rdata` and `idata` methods, respectively.

```
Particle<2, 2> p;

p.pos(0) = 1.0;
p.pos(1) = 2.0;
p.pos(2) = 3.0;
p.id() = 1;
p.cpu() = 0;

// p.rdata(0) is the first extra real component, not the
// first real component overall
p.rdata(0) = 5.0;
p.rdata(1) = 5.0;

// and likewise for p.idata(0);
p.rdata(0) = 17;
p.idata(1) = -64;
```

11.2 The ParticleContainer

One particle by itself is not very useful. To do real calculations, a collection of particles needs to be defined, and the location of the particles within the AMR hierarchy (and the corresponding MPI process) needs to be tracked as the particle positions change. To do this, we provide the `ParticleContainer` class:

```
ParticleContainer<3, 2, 4, 4> mypc;
```

11.2.1 Arrays-of-Structs and Structs-of-Arrays

Like the `Particle` class itself, the `ParticleContainer` class is templated. The first two template parameters have the same meaning as before: they define the number of each type of variables that the particles in this container will store. Particles added to the container are stored in the Array-of-Structs (AoS) style. In addition, there are two more optional template parameters that allow the user to specify additional particle variables that will be stored in Struct-of-Array (SoA) form. The difference between Array-of-Struct and Struct-of-Array data is in how the data is laid out in memory. For the AoS data, all the variables associated with particle 1 are next to each other in memory, followed by all the variables associated with particle 2, and so on. For variables stored in SoA style, all the particle data for a given component is next to each other in memory, and each component is stored in a separate array. For convenience, we (arbitrarily) refer to the components in the particle struct as particle *data*, and components stored in the Struct-of-Arrays as particle *attributes*. See the figure *below* for an illustration.

To see why the distinction between AoS and SoA data is important, consider the following extreme case. Say you have particles that carry 100 different components, but that most of the time, you only need to do calculations involving 3 of them (say, the particle positions) at once. In this case, storing all 100 particle variables in the particle struct is clearly inefficient, since most of the time you are reading 97 extra variables into cache that you will never use. By splitting up the particle variables into stuff that gets used all the time (stored in the AoS) and stuff that only gets used infrequently (stored in the SoA), you can in principle achieve much better cache reuse. Of course, the usage pattern

Array-of-Structs



Struct-of-Arrays



Fig. 11.1: An illustration of how the particle data for a single tile is arranged in memory. This particle container has been defined with `NStructReal = 1`, `NStructInt = 2`, `NArrayReal = 2`, and `NArrayInt = 2`. In this case, each tile in the particle container has five arrays: one with the particle struct data, two additional real arrays, and two additional integer arrays. In the tile shown, there are only 2 particles. We have labelled the extra real data member of the particle struct to be `mass`, while the extra integer members of the particle struct are labeled `p`, and `s`, for “phase” and “state”. The variables in the real and integer arrays are labelled `foo`, `bar`, `l`, and `n`, respectively. We have assumed that the particles are double precision.

of your application likely won't be so clear-cut. Flexibility in how the particle data is stored also makes it easier to interface between AMReX and already-existing Fortran subroutines.

Note that while “extra” particle data can be stored in either the SoA or AoS style, the particle positions and id numbers are **always** stored in the particle structs. This is because these particle variables are special and used internally by AMReX to assign the particles to grids and to mark particles as valid or invalid, respectively.

11.2.2 Constructing ParticleContainers

A particle container is always associated with a particular set of AMR grids and a particular set of DistributionMaps that describes which MPI processes those grids live on. For example, if you only have one level, you can define a `ParticleContainer` to store particles on that level using the following constructor:

```
ParticleContainer (const Geometry & geom,  
                  const DistributionMapping & dmap,  
                  const BoxArray & ba);
```

Or, if you have multiple levels, you can use following constructor instead:

```
ParticleContainer (const Vector<Geometry> & geom,  
                  const Vector<DistributionMapping> & dmap,  
                  const Vector<BoxArray> & ba,  
                  const Vector<int> & rr);
```

Note the set of grids used to define the `ParticleContainer` doesn't have to be the same set used to define the simulation's mesh data. However, it is often desirable to have the two hierarchies track each other. If you are using an `AmrCore` class in your simulation (see the Chapter on [AmrCore Source Code](#)), you can achieve this by using the `AmrParticleContainer` class. The constructor for this class takes a pointer to your `AmrCore` derived class, instead:

```
AmrTracerParticleContainer (AmrCore* amr_core);
```

In this case, the `Vector<BoxArray>` and `Vector<DistributionMap>` used by your `ParticleContainer` will be updated automatically to match those in your `AmrCore`.

The `ParticleContainer` stores the particle data in a manner prescribed by the set of AMR grids used to define it. If tiling is turned off, then every grid has its own Array-of-Structs and Struct-of-Arrays. Which AMR grid a particle is assigned to is determined by examining its position and binning it, using the domain left edge as an offset. By default, a particle is assigned to the finest level that contains its position, although this behavior can be tweaked if desired. When tiling is enabled, then each *tile* gets its own Struct-of-Arrays and Array-of-Structs instead. Note that this is different than what happens with mesh data. With mesh data, the tiling is strictly logical; the data is laid out in memory the same whether tiling is turned on or off. With particle data, however, the particles are actually stored in different arrays when tiling is enabled. As with mesh data, the particle tile size can be tuned so that an entire tile's worth of particles will fit into a cache line at once.

Once the particles move, their data may no longer be in the right place in the container. They can be reassigned by calling the `Redistribute()` method of `ParticleContainer`. After calling this method, all the particles will be moved to their proper places in the container, and all invalid particles (particles with id set to -1) will be removed. All the MPI communication needed to do this happens automatically.

Application codes will likely want to create their own derived `ParticleContainer` class that specializes the template parameters and adds additional functionality, like setting the initial conditions, moving the particles, etc. See the `amrex/Tutorials/Particles` for examples of this.

11.3 Initializing Particle Data

In the following code snippet, we demonstrate how to set particle initial conditions for both SoA and AoS data. We loop over all the tiles using `MFIter`, and add as many particles as we want to each one.

```
for (MFIter mfi = MakeMFIter(lev); mfi.isValid(); ++mfi) {

    // ``particles'' starts off empty
    auto& particles = GetParticles(lev) [std::make_pair(mfi.index(),
                                                       mfi.LocalTileIndex())];

    ParticleType p;
    p.id()    = ParticleType::NextID();
    p.cpu()   = ParallelDescriptor::MyProc();
    p.pos(0)  = ...
    etc...

    // AoS real data
    p.rdata(0) = ...
    p.rdata(1) = ...

    // AoS int data
    p.idata(0) = ...
    p.idata(1) = ...

    // Particle real attributes (SoA)
    std::array<double, 2> real_attribs;
    real_attribs[0] = ...
    real_attribs[1] = ...

    // Particle int attributes (SoA)
    std::array<int, 2> int_attribs;
    int_attribs[0] = ...
    int_attribs[1] = ...

    particles.push_back(p);
    particles.push_back_real(real_attribs);
    particles.push_back_int(int_attribs);

    // ... add more particles if desired ...
}
```

Often, it makes sense to have each process only generate particles that it owns, so that the particles are already in the right place in the container. In general, however, users may need to call `Redistribute()` after adding particles, if the processes generate particles they don't own (for example, if the particle positions are perturbed from the cell centers and thus end up outside their parent grid).

11.4 Iterating over Particles

To iterate over the particles on a given level in your container, you can use the `ParIter` class, which comes in both `const` and non-`const` flavors. For example, to iterate over all the AoS data:

```
using MyParIter = ConstParIter<2*BL_SPACEDIM>;
for (MyParIter pti(pc, lev); pti.isValid(); ++pti) {
```

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```

const auto& particles = pti.GetArrayOfStructs();
for (const auto& p : particles) {
    // do stuff with p...
}
}

```

The outer loop will execute once every grid (or tile, if tiling is enabled) *that contains particles*; grids or tiles that don't have any particles will be skipped. You can also access the SoA data using the *ParIter* as follows:

```

using MyParIter = ParIter<0, 0, 2, 2>;
for (MyParIter pti(pc, lev); pti.isValid(); ++pti) {
    auto& particle_attributes = pti.GetStructOfArrays();
    Vector<Real>& real_comp0 = particle_attributes.GetRealData(0);
    Vector<int>& int_compl = particle_attributes.GetIntData(1);
    for (int i = 0; i < pti.numParticles; ++i) {
        // do stuff with your SoA data...
    }
}

```

11.5 Passing particle data into Fortran routines

Because the AMReX particle struct is a Plain-Old-Data type, it is interoperable with Fortran when the `bind(C)` attribute is used. It is therefore possible to pass a grid or tile worth of particles into fortran routines for processing, instead of iterating over them in C++. You can also define a Fortran derived type that is equivalent to C struct used for the particles. For example:

```

use amrex_fort_module, only: amrex_particle_real
use iso_c_binding , only: c_int

type, bind(C) :: particle_t
    real(amrex_particle_real) :: pos(3)
    real(amrex_particle_real) :: vel(3)
    real(amrex_particle_real) :: acc(3)
    integer(c_int) :: id
    integer(c_int) :: cpu
end type particle_t

```

is equivalent to a particle struct you get with `Particle<6, 0>`. Here, `amrex_particle_real` is either single or doubled precision, depending on whether `USE_SINGLE_PRECISION_PARTICLES` is TRUE or not. We recommend always using this type in Fortran routines that work on particle data to avoid hard-to-debug incompatibilities between floating point types.

11.6 Interacting with Mesh Data

It is common to want to have the mesh communicate information to the particles and vice versa. For example, in Particle-in-Cell calculations, the particles deposit their charges onto the mesh, and later, the electric fields computed on the mesh are interpolated back to the particles. Below, we show examples of both these sorts of operations.

```

Ex.FillBoundary(gm.periodicity());
Ey.FillBoundary(gm.periodicity());
Ez.FillBoundary(gm.periodicity());

```

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```

for (MyParIter pti(MyPC, lev); pti.isValid(); ++pti) {
    const Box& box = Ex[pti].validBox();

    const auto& particles = pti.GetArrayOfStructs();
    int nstride = particles.dataShape().first;
    const long np = pti.numParticles();

    const FArrayBox& exfab = Ex[pti];
    const FArrayBox& eyfab = Ey[pti];
    const FArrayBox& ezzfab = Ez[pti];

    interpolate_cic(particles.data(), nstride, np,
                     exfab.dataPtr(), eyfab.dataPtr(), ezzfab.dataPtr(),
                     box.loVect(), box.hiVect(), plo, dx, &ng);
}

```

Here, `interpolate_cic` is a Fortran subroutine that actually performs the interpolation on a single box. `Ex`, `Ey`, and `Ez` are MultiFabs that contain the electric field data. These MultiFabs must be defined with the correct number of ghost cells to perform the desired type of interpolation, and we call `FillBoundary` prior to the Fortran call so that those ghost cells will be up-to-date.

In this example, we have assumed that the `ParticleContainer` `MyPC` has been defined on the same grids as the electric field MultiFabs, so that we use the `ParIter` to index into the MultiFabs to get the data associated with current tile. If this is not the case, then an additional copy will need to be performed. However, if the particles are distributed in an extremely uneven fashion, it is possible that the load balancing improvements associated with the two-grid approach are worth the cost of the extra copy.

The inverse operation, in which the particles communicate data *to* the mesh, is quite similar:

```

rho.setVal(0.0, ng);
for (MyParIter pti(*this, lev); pti.isValid(); ++pti) {
    const Box& box = rho[pti].validbox();

    const auto& particles = pti.GetArrayOfStructs();
    int nstride = particles.dataShape().first;
    const long np = pti.numParticles();

    FArrayBox& rhofab = (*rho[lev])[pti];

    deposit_cic(particles.data(), nstride, np, rhofab.dataPtr(),
                box.loVect(), box.hiVect(), plo, dx);
}

rho.SumBoundary(gm.periodicity());

```

As before, we loop over all our particles, calling a Fortran routine that deposits them on to the appropriate `FArrayBox` `rhofab`. The `rhofab` must have enough ghost cells to cover the support of all the particles associated with them. Note that we call `SumBoundary` instead of `FillBoundary` after performing the deposition, to add up the charge in the ghost cells surrounding each Fab into the corresponding valid cells.

For a complete example of an electrostatic PIC calculation that includes static mesh refinement, please see `amrex/Tutorials/Particles/ElectrostaticPIC`.

11.7 Short Range Forces

In a PIC calculation, the particles don't interact with each other directly; they only see each other through the mesh. An alternative use case is particles that exert short-range forces on each other. In this case, beyond some cut-off distance, the particles don't interact with each other and therefore don't need to be included in the force calculation. Our approach to these kind of particles is to fill “neighbor buffers” on each tile that contain copies of the particles on neighboring tiles that are within some number of cells N_g of the tile boundaries. See Fig. 11.2, below for an illustration. By choosing the number of ghost cells to match the interaction radius of the particles, you can capture all of the neighbors that can possibly influence the particles in the valid region of the tile. The forces on the particles on different tiles can then be computed independently of each other using a variety of methods.

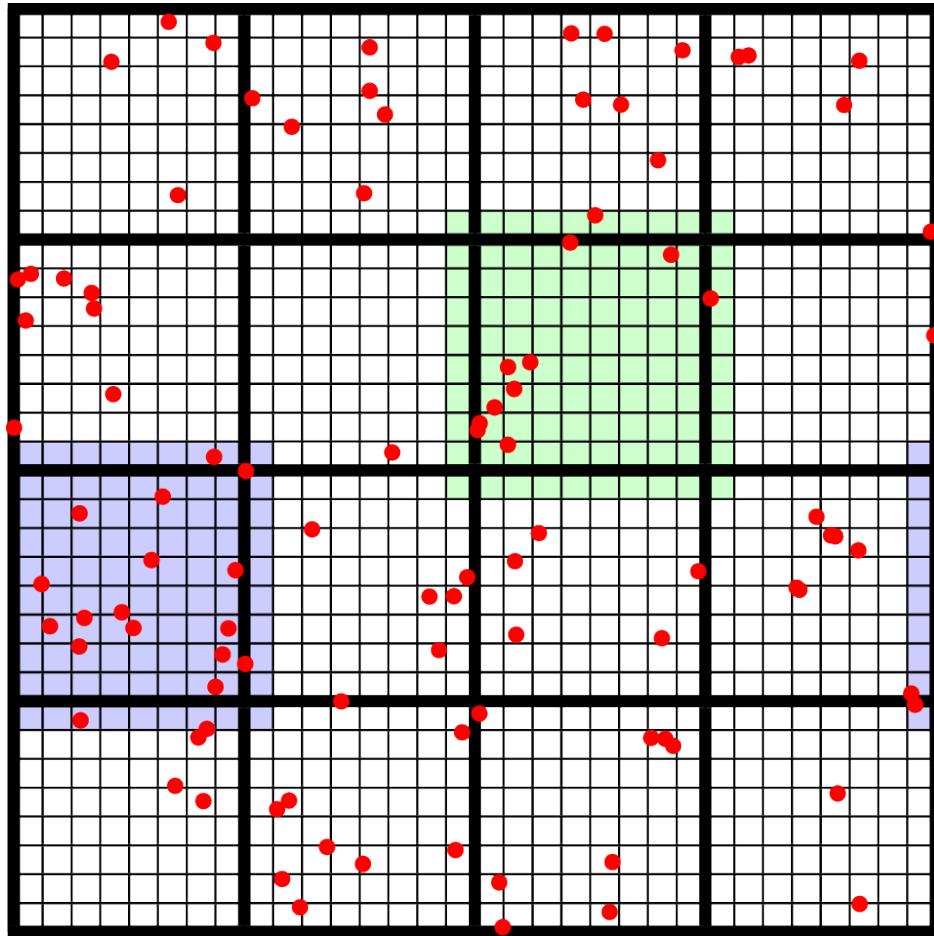


Fig. 11.2: : An illustration of filling neighbor particles for short-range force calculations. Here, we have a domain consisting of one 32×32 grid, broken up into 8×8 tiles. The number of ghost cells is taken to be 1. For the tile in green, particles on other tiles in the entire shaded region will be copied and packed into the green tile's neighbor buffer. These particles can then be included in the force calculation. If the domain is periodic, particles in the grown region for the blue tile that lie on the other side of the domain will also be copied, and their positions will be modified so that a naive distance calculation between valid particles and neighbors will be correct.

For a `ParticleContainer` that does this neighbor finding, please see `NeighborParticleContainer` in `amrex/Src/Particles/AMReX_NeighborParticleContainer.H`. This `ParticleContainer` has additional methods called `fillNeighbors()` and `clearNeighbors()` that fill the `neighbors` data structure with copies of the proper particles. A tutorial that uses these features is available at `amrex/Tutorials/`

Particles/ShortRangeParticles. This tutorial computes the forces on a given tile via direct summation by passing the real and neighbor particles into a Fortran subroutine, as follows:

```
void ShortRangeParticleContainer::computeForces() {
    for (MyParIter pti(*this, lev); pti.isValid(); ++pti) {
        AoS& particles = pti.GetArrayOfStructs();
        int Np = particles.size();
        PairIndex index(pti.index(), pti.LocalTileIndex());
        int Nn = neighbors[index].size() / pdata_size;
        amrex_compute_forces(particles.data(), &Np,
                             neighbors[index].dataPtr(), &Nn);
    }
}
```

Alternatively, one can avoid doing a direct N^2 summation over the particles on a tile by binning the particles by cell and building a neighbor list. A tutorial that demonstrates this process is available at [amrex/Tutorials/Particles/NeighborList](#). The data structure used to represent the neighbor lists is illustrated in Fig. 11.3.



Fig. 11.3: : An illustration of the neighbor list data structure used by AMReX. The list for each tile is represented by an array of integers. The first number in the array is the number of real (i.e., not in the neighbor buffers) collision partners for the first particle on this tile, while the second is the number of collision partners from nearby tiles in the neighbor buffer. Based on the number of collision partners, the next several entries are the indices of the collision partners in the real and neighbor particle arrays, respectively. This pattern continues for all the particles on this tile.

This array can then be used to compute the forces on all the particles in one scan. Users can define their own `NeighborParticleContainer` subclasses that have their own collision criteria by overloading the virtual `check_pair` function. For an example of this in action, please see the `NeighborList` Tutorial.

11.8 Particle IO

AMReX provides routines for writing particle data to disk for analysis, visualization, and for checkpoint / restart. The most important methods are the `WritePlotFile`, `Checkpoint`, and `Restart` methods of `ParticleContainer`, which all use a parallel-aware binary file format for reading and writing particle data on a grid-by-grid basis. These methods are designed to complement the functions in `AMReX_PlotFileUtil.H` for performing mesh data IO. For example:

```
WriteMultiLevelPlotfile("plt00000", output_levs, GetVecOfConstPtrs(output),
                       varnames, geom, 0.0, level_steps, outputRR);
pc.Checkpoint("plt00000", "particle0");
```

will create a plot file called “plt00000” and write the mesh data in `output` to it, and then write the particle data in a subdirectory called “particle0”. There is also the `WriteAsciiFile` method, which writes the particles in a human-readable text format. This is mainly useful for testing and debugging.

The binary file format is currently readable by `yt`. In addition, there is a Python conversion script in `amrex/Tools/Py_util/amrex_particles_to_vtp` that can convert both the ASCII and the binary particle files to

a format readable by Paraview. See the chapter on [*Visualization*](#) for more information on visualizing AMReX datasets, including those with particles.

FORTRAN INTERFACE

The core of AMReX is written in C++. For Fortran users who want to write all of their programs in Fortran, AMReX provides Fortran interfaces around most of functionalities except for the `AmrLevel` class (see the chapter on [Amr Source Code](#)) and particles (see the chapter on [Particles](#)). We should not confuse the Fortran interface in this chapter with the Fortran kernel functions called inside `MFIter` loops in codes (see the section on [Fortran, C and C++ Kernels](#)). For the latter, Fortran is used in some sense as a domain-specific language with native multi-dimensional arrays, whereas here Fortran is used to drive the whole application code. In order to better understand AMReX, Fortran interface users should read the rest of the documentation except for the Chapters on [Amr Source Code & Particles](#).

12.1 Getting Started

We have discussed AMReX’s build systems in the chapter on [Building AMReX](#). To build with GNU Make, we need to include the Fortran interface source tree into the make system. The source codes for the Fortran interface are in `amrex/Src/F_Interfaces` and there are several sub-directories. The “Base” directory includes sources for the basic functionality, the “`AmrCore`” directory wraps around the `AmrCore` class (see the chapter on [AmrCore Source Code](#)), and the “Octree” directory adds support for octree type of AMR grids. Each directory has a “`Make.package`” file that can be included in make files (see `amrex/Tutorials/Basic>HelloWorld_F` and `amrex/Tutorials/Amr/Advection_F` for examples). The `libamrex` approach includes the Fortran interface by default. The CMake approach does not support the Fortran interface yet.

A simple example can be found at `amrex/Tutorials/Basic>HelloWorld_F/`. The source code is shown below in its entirety.

```
program main
  use amrex_base_module
  implicit none
  call amrex_init()
  if (amrex_parallel_ioprocessor()) then
    print *, "Hello world!"
  end if
  call amrex_finalize()
end program main
```

To access the AMReX Fortran interfaces, we can use these three modules, `amrex_base_module` for the basics functionalities (Section 2), `amrex_amrcore_module` for AMR support (Section 3) and `amrex_octree_module` for octree style AMR (Section 4).

12.2 The Basics

Module `amrex_base_module` is a collection of various Fortran modules providing interfaces to most of the basics of AMReX C++ library (see the chapter on *Basics*). These modules shown in this section can be used without being explicitly included because they are included by `amrex_base_module`.

The spatial dimension is an integer parameter `amrex_spacedim`. We can also use the `AMREX_SPACEDIM` macro in preprocessed Fortran codes (e.g., .F90 files) just like in the C++ codes. Unlike in C++, the convention for AMReX Fortran interface is that coordinate direction index starts at 1.

There is an integer parameter `amrex_real`, a Fortran kind parameter for `real`. Fortran `real` (`amrex_real`) corresponds to `amrex::Real` in C++, which is either double or single precision depending the setting of precision.

The module `amrex_parallel_module` (`amrex/Src/F_Interfaces/Base/AMReX_parallel_mod.F90`) includes wrappers to the `ParallelDescriptor` namespace, which is in turn a wrapper to the parallel communication library used by AMReX (e.g. MPI).

The module `amrex_parmparse_module` (`amrex/Src/Base/AMReX_parmparse_mod.F90`) provides interface to `ParmParse` (see the section on *ParmParse*). Here are some examples.

```
type(amrex_parmparse) :: pp
integer :: n_cell, max_grid_size
call amrex_parmparse_build(pp)
call pp%get("n_cell", n_cell)
max_grid_size = 32 ! default size
call pp%query("max_grid_size", max_grid_size)
call amrex_parmpase_destroy(pp) ! optional if compiler supports finalization
```

Finalization is a Fortran 2003 feature that some compilers may not support. For those compilers, we must explicitly destroy the objects, otherwise there will be memory leaks. This applies to many other derived types.

`amrex_box` is a derived type in `amrex_box_module` (`amrex/Src/F_Interfaces/Base/AMReX_box_mod.F90`). It has three members, `lo` (lower corner), `hi` (upper corner) and `nodal` (logical flag for index type).

`amrex_geometry` is a wrapper for the `Geometry` class containing information for the physical domain. Below is an example of building it.

```
integer :: n_cell
type(amrex_box) :: domain
type(amrex_geometry) : geom
! n_cell = ...
! Define a single box covering the domain
domain = amrex_box((/0,0,0/), (/n_cell-1, n_cell-1, n_cell-1/))
! This defines a amrex_geometry object.
call amrex_geometry_build(geom, domain)
!
! ...
!
call amrex_geometry_destroy(geom)
```

`amrex_boxarray` (`amrex/Src/F_Interfaces/Base/AMReX_boxarray_mod.F90`) is a wrapper for the `BoxArray` class, and `amrex_distromap` (`amrex/Src/F_Interfaces/Base/AMReX_distromap_mod.F90`) is a wrapper for the `DistributionMapping` class. Here is an example of building a `BoxArray` and a `DistributionMapping`.

```
integer :: n_cell
type(amrex_box) :: domain
```

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```

type(amrex_boxarray) : ba
type(amrex_distromap) :: dm
! n_cell = ...
! Define a single box covering the domain
domain = amrex_box((/0,0,0/), (/n_cell-1, n_cell-1, n_cell-1/))
! Initialize the boxarray "ba" from the single box "bx"
call amrex_boxarray_build(ba, domain)
! Break up boxarray "ba" into chunks no larger than "max_grid_size"
call ba%maxSize(max_grid_size)
! Build a DistributionMapping for the boxarray
call amrex_distromap_build(dm, ba)
!
! ...
!
call amrex_distromap_distromap(dm)
call amrex_boxarray_destroy(ba)

```

Given `amrex_boxarray` and `amrex_distromap`, we can build `amrex_multifab`, a wrapper for the `MultiFab` class, as follows.

```

integer :: ncomp, nghost
type(amrex_boxarray) : ba
type(amrex_distromap) :: dm
type(amrex_multifab) :: mf, ndmf
! Build amrex_boxarray and amrex_distromap
! ncomp = ...
! nghost = ...
!
! ...
! Build amrex_multifab with ncomp component and nghost ghost cells
call amrex_multifab_build(mf, ba, dm, ncomp, nghost)
! Build a nodal multifab
call amrex_multifab_build(ndmf, ba, dm, ncomp, nghost, (/ .true., .true., .true. /))
!
! ...
!
call amrex_multifab_destroy(mf)
call amrex_multifab_destroy(ndmf)

```

There are many type-bound procedures for `amrex_multifab`. For example

```

ncomp ! Return the number of components
nghost ! Return the number of ghost cells
setval ! Set the data to the given value
copy ! Copy data from given amrex_multifab to this amrex_multifab

```

Note that the `copy` function here only works on copying data from another `amrex_multifab` built with the same `amrex_distromap`, like the `MultiFab::Copy` function in C++. `amrex_multifab` also has two parallel communication procedures, `fill_boundary` and `parallel_copy`. Their interface and usage are very similar to functions `FillBoundary` and `ParallelCopy` for `MultiFab` in C++.

```

type(amrex_geometry) :: geom
type(amrex_multifab) :: mf, mfsrc
!
call mf%fill_boundary(geom) ! Fill all components
call mf%fill_boundary(geom, 1, 3) ! Fill 3 components starting with component 1

call mf%parallel_copy(mfsrc, geom) ! Parallel copy from another multifab

```

It should be emphasized that the component index for `amrex_multifab` starts with 1 following Fortran convention. This is different from the C++ part of AMReX.

AMReX provides a Fortran interface to `MFIter` for iterating over the data in `amrex_multifab`. The Fortran type for this is `amrex_mfiter`. Here is an example of using `amrex_mfiter` to loop over `amrex_multifab` with tiling and launch a kernel function.

```
integer :: plo(4), phi(4)
type(amrex_box) :: bx
real(amrex_real), contiguous, dimension(:,:,:,:), pointer :: po, pn
type(amrex_multifab) :: old_phi, new_phi
type(amrex_mfiter) :: mfi
! Define old_phi and new_phi ...
! In this example they are built with the same boxarray and distromap.
! And they have the same number of ghost cells and 1 component.
call amrex_mfiter_build(mfi, old_phi, tiling=.true.)
do while (mfi%next())
    bx = mfi%tilebox()
    po => old_phi%dataptr(mfi)
    pn => new_phi%dataptr(mfi)
    plo = lbound(po)
    phi = ubound(po)
    call update_phi(bx%lo, bx&hi, po, pn, plo, phi)
end do
call amrex_mfiter_destroy(mfi)
```

Here procedure `update_phi` is

```
subroutine update_phi (lo, hi, pold, pnew, plo, phi)
    integer, intent(in) :: lo(3), hi(3), plo(3), phi(3)
    real(amrex_real), intent(in) :: pold(plo(1):phi(1),plo(2):phi(2),plo(3):phi(3))
    real(amrex_real), intent(inout) :: pnew(plo(1):phi(1),plo(2):phi(2),plo(3):phi(3))
    ! ...
end subroutine update_phi
```

Note that `amrex_multifab`'s procedure `dataptr` takes `amrex_mfiter` and returns a 4-dimensional Fortran pointer. For performance, we should declare the pointer as `contiguous`. In C++, the similar operation returns a reference to `FArrayBox`. However, `FArrayBox` and Fortran pointer have a similar capability of containing array bound information. We can call `lbound` and `ubound` on the pointer to return its lower and upper bounds. The first three dimensions of the bounds are spatial and the fourth is for the number of component.

Many of the derived Fortran types in (e.g., `amrex_multifab`, `amrex_boxarray`, `amrex_distromap`, `amrex_mfiter`, and `amrex_geometry`) contain a type (`c_ptr`) that points a C++ object. They also contain a logical type indicating whether or not this object owns the underlying object (i.e., responsible for deleting the object). Due to the semantics of Fortran, one should not return these types with functions. Instead we should pass them as arguments to procedures (preferably with `intent` specified). These five types all have assignment(`=`) operator that performs a shallow copy. After the assignment, the original objects still owns the data and the copy is just an alias. For example,

```
type(amrex_multifab) :: mf1, mf2
call amrex_multifab_build(mf1, ...)
call amrex_multifab_build(mf2, ...)
! At this point, both mf1 and mf2 are data owners
mf2 = mf1 ! This will destroy the original data in mf2.
           ! Then mf2 becomes a shallow copy of mf1.
           ! mf1 is still the owner of the data.
call amrex_multifab_destroy(mf1)
```

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```
! mf2 no longer contains a valid pointer because mf1 has been destroyed.
call amrex_multifab_destroyed(mf2) ! But we still need to destroy it.
```

If we need to transfer the ownership, `amrex_multifab`, `amrex_boxarray` and `amrex_distromap` provide type-bound move procedure. We can use it as follows

```
type(amrex_multifab) :: mf1, mf2
call amrex_multifab_build(mf1, ...)
call mf2%move(mf1) ! mf2 is now the data owner and mf1 is not.
call amrex_multifab_destroy(mf1)
call amrex_multifab_destroyed(mf2)
```

`amrex_multifab` also has a type-bound swap procedure for exchanging the data.

AMReX also provides `amrex_plotfile_module` for writing plotfiles. The interface is similar to the C++ versions.

12.3 Amr Core Infrastructure

The module `amrex_amr_module` provides interfaces to AMR core infrastructure. With AMR, the main program might look like below,

```
program main
  use amrex_amr_module
  implicit none
  call amrex_init()
  call amrex_amrcore_init()
  call my_amr_init() ! user's own code, not part of AMReX
  !
  call my_amr_finalize() ! user's own code, not part of AMReX
  call amrex_amrcore_finalize()
  call amrex_finalize()
end program main
```

Here we need to call `amrex_amrcore_init` and `amrex_amrcore_finalize`. And usually we need to call application code specific procedures to provide some “hooks” needed by AMReX. In C++, this is achieved by using virtual functions. In Fortran, we need to call

```
subroutine amrex_init_virtual_functions (mk_lev_scrtch, mk_lev_crse, &
                                         mk_lev_re, clr_lev, err_est)

  ! Make a new level from scratch using provided boxarray and distromap
  ! Only used during initialization.
  procedure(amrex_make_level_proc) :: mk_lev_scrtch
  ! Make a new level using provided boxarray and distromap, and fill
  ! with interpolated coarse level data.
  procedure(amrex_make_level_proc) :: mk_lev_crse
  ! Remake an existing level using provided boxarray and distromap,
  ! and fill with existing fine and coarse data.
  procedure(amrex_make_level_proc) :: mk_lev_re
  ! Delete level data
  procedure(amrex_clear_level_proc) :: clr_lev
  ! Tag cells for refinement
  procedure(amrex_error_est_proc) :: err_est
end subroutine amrex_init_virtual_functions
```

We need to provide five functions and these functions have three types of interfaces:

```
subroutine amrex_make_level_proc (lev, time, ba, dm) bind(c)
  import
  implicit none
  integer, intent(in), value :: lev
  real(amrex_real), intent(in), value :: time
  type(c_ptr), intent(in), value :: ba, dm
end subroutine amrex_make_level_proc

subroutine amrex_clear_level_proc (lev) bind(c)
  import
  implicit none
  integer, intent(in) , value :: lev
end subroutine amrex_clear_level_proc

subroutine amrex_error_est_proc (lev, tags, time, tagval, clearval) bind(c)
  import
  implicit none
  integer, intent(in), value :: lev
  type(c_ptr), intent(in), value :: tags
  real(amrex_real), intent(in), value :: time
  character(c_char), intent(in), value :: tagval, clearval
end subroutine amrex_error_est_proc
```

Tutorials/Amr/Advection_F/Source/my_amr_mod.F90 shows an example of the setup process. The user provided procedure (amrex_error_est_proc) has a tags argument that is of type c_ptr and its value is a pointer to a TagBoxArray object. We need to convert this into a Fortran amrex_tagboxarray object.

```
type(amrex_tagboxarray) :: tag
tag = tags
```

The module amrex_fillpatch_module provides interface to C++ functions FillPatchSinglelevel and FillPatchTwoLevels. To use it, the application code needs to provide procedures for interpolation and filling physical boundaries. See Tutorials/Amr/Advection_F/Source/fillpatch_mod.F90 for an example.

Module amrex_fluxregister_module provides interface to FluxRegister (see the section on [Using FluxRegisters](#)). Its usage is demonstrated in the tutorial at Tutorials/Amr/Advection_F/.

12.4 Octree

In AMReX, the union of fine level grids is properly contained within the union of coarse level grids. There are no required direct parent-child connections between levels. Therefore, grids in AMReX in general cannot be represented by trees. Nevertheless, octree type grids are supported via Fortran interface, because grids are more general than octree grids. A tutorial example using amrex_octree_module (`amrex/Src/F_Interfaces/Octree/AMReX_octree_mod.f90`) is available at `amrex/Tutorials/Amr/Advection_octree_F/`. Procedures `amrex_octree_init` and `amrex_octree_finalize` must be called as follows,

```
program main
  use amrex_amrcore_module
  use amrex_octree_module
  implicit none
  call amrex_init()
  call amrex_octree_int() ! This should be called before amrex_amrcore_init.
  call amrex_amrcore_init()
```

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```

call my_amr_init()           ! user's own code, not part of AMReX
!
call my_amr_finalize()      ! user's own code, not part of AMReX
call amrex_amrcore_finalize()
call amrex_octree_finalize()
call amrex_finalize()
end program main

```

By default, the grid size is 8^3 , and this can be changed via ParmParse parameter `amr.max_grid_size`. The module `amrex_octree_module` provides `amrex_octree_iter` that can be used to iterate over leaves of octree. For example,

```

type(amrex_octree_iter) :: oti
type(multifab) :: phi_new(*)   ! one multifab for each level
integer :: ilev, igrd
type(amrex_box) :: bx
real(amrex_real), contiguous, pointer, dimension(:,:,:,:,:) :: pout
call amrex_octree_iter_build(oti)
do while(oti%next())
    ilev = oti%level()
    igrd = oti%grid_index()
    bx   = oti%box()
    pout => phi_new(ilev)%dataptr(igrd)
    !
end do
call amrex_octree_iter_destroy(oti)

```


EMBEDDED BOUNDARIES

13.1 Overview of Embedded Boundary Description

For computations with complex geometries, AMReX provides data structures and algorithms to employ an embedded boundary (EB) approach to PDE discretizations. In this approach, the underlying computational mesh is uniform and block-structured, but the boundary of the irregular-shaped computational domain conceptually cuts through this mesh. Each cell in the mesh becomes labeled as regular, cut or covered, and the finite-volume based discretization methods traditionally used in AMReX applications can be modified to incorporate these cell shapes. See [Fig. 13.1](#) for an illustration.



Fig. 13.1: : In the embedded boundary approach to discretizing PDEs, the (uniform) rectangular mesh is cut by the irregular shape of the computational domain. The cells in the mesh are label as regular, cut or covered.

Because this is a relatively simple grid generation technique, computational meshes for rather complex geometries can be generated quickly and robustly. However, the technique can produce arbitrarily small cut cells in the domain. In practice such small cells can have significant impact on the robustness and stability of traditional finite volume methods. In this chapter we overview a class of approaches to deal with this “small cell” problem in a robust and efficient way, and discuss the tools and data that AMReX provides in order to implement them.

Note that in a completely general implementation of the EB approach, there would be no restrictions on the shape or complexity of the EB surface. With this generality comes the possibility that the process of “cutting” the cells results in a single (i, j, k) cell being broken into multiple cell fragments. The current release of AMReX does not support multi-valued cells, thus there is a practical restriction on the complexity of domains (and numerical algorithms) supported.

This chapter discusses the EB tools, data structures and algorithms currently supported by AMReX to enable the construction of discretizations of conservation law systems. The discussion will focus on general requirements associated with building fluxes and taking divergences of them to advance such systems. We also give examples of how to initialize the geometry data structures and access them to build the numerical difference operators. Finally we present EB support of linear solvers.

13.1.1 Finite Volume Discretizations

Consider a system of PDEs to advance a conserved quantity U with fluxes F :

$$\frac{\partial U}{\partial t} + \nabla \cdot F = 0. \quad (13.1)$$

A conservative, finite volume discretization starts with the divergence theorem

$$\int_V \nabla \cdot F dV = \int_{\partial V} F \cdot n dA.$$

In an embedded boundary cell, the “conservative divergence” is discretized (as $D^c(F)$) as follows

$$D^c(F) = \frac{1}{\kappa h} \left(\sum_{d=1}^D (F_{d,\text{hi}} \alpha_{d,\text{hi}} - F_{d,\text{lo}} \alpha_{d,\text{lo}}) + F^{EB} \alpha^{EB} \right). \quad (13.2)$$

Geometry is discretely represented by volumes ($V = \kappa h^d$) and apertures ($A = \alpha h^{d-1}$), where h is the (uniform) mesh spacing at that AMR level, κ is the volume fraction and α are the area fractions. Without multivalued cells the volume fractions, area fractions and cell and face centroids (see Table 13.1) are the only geometric information needed to compute second-order fluxes centered at the face centroids, and to infer the connectivity of the cells. Cells are connected if adjacent on the Cartesian mesh, and only via coordinate-aligned faces on the mesh. If an aperture, $\alpha = 0$, between two cells, they are not directly connected to each other.

Table 13.1: Illustration of embedded boundary cutting a two-dimensional cell.

| | |
|---|------------------------------|
| | |
| <p>A typical two-dimensional uniform cell that is cut by the embedded boundary. The grey area represents the region excluded from the calculation. The portion of the cell faces faces (labelled with A) through which fluxes flow are the “uncovered” regions of the full cell faces. The volume (labelled V) is the uncovered region of the interior.</p> | <p>Fluxes in a cut cell.</p> |

13.1.2 Small Cells And Stability

In the context of time-explicit advance methods for, say hyperbolic conservation laws, a naive discretization in time of (13.1) using (13.2),

$$U^{n+1} = U^n - \delta t D^c(F)$$

would have a time step constraint $\delta t \sim h\kappa^{1/D}/V_m$, which goes to zero as the size of the smallest volume fraction κ in the calculation. Since EB volume fractions can be arbitrarily small, this is an unacceptable constraint. One way to remedy this is to create “non-conservative” approximation to the divergence D^{nc} , which at a cell i , can be formed as an average of the conservative divergences in the neighborhood, N_i , of i .

$$D^{nc}(F)_i = \frac{\sum_{j \in N_i} \kappa_j D(F)_j}{\sum_{j \in N_i} \kappa_j}$$

Incorporating this form, the solution can be updated using a *hybrid divergence*, $D^H(F) = \kappa D^c(F) + (1 - \kappa) D^{nc}$:

$$U^{n+1,*} = U^n - \delta t D^H(F)$$

However, we would like our finite-volume scheme to strictly conserve the field quantities over the domain. To enforce this, we calculate δM , the mass gained or lost by not using D^c directly,

$$\delta M_i = \kappa(1 - \kappa)(D^c(F)_i - D^{nc}(F)_i)$$

This “excess material” (mass, if $U = \rho$) can be *redistributed* in a time-explicit fashion to neighboring cells, $\mathbf{j} \in N_i$:

$$\delta M_i = \sum_{\mathbf{j} \in N_i} \delta M_{j,i}.$$

in order to preserve strict conservation over N_i .

Note that the physics at hand may impact the optimal choice of precisely how the excess mass is distributed in this fashion. We introduce a weighting for redistribution, W ,

$$\delta M_{j,i} = \frac{\delta M_i \kappa_j W_j}{\sum_{\mathbf{k} \in N_i} \kappa_k W_k} \quad (13.3)$$

For all $\mathbf{j} \in N_i$,

$$U_j^{n+1} = U_j^{n+1,*} + \frac{\delta M_i W_j}{\sum_{\mathbf{k} \in N_i} \kappa_k W_k}.$$

Typically, the redistribution neighborhood for each cell is one that can be reached via a monotonic path in each coordinate direction of unit length (see, e.g., Fig. 13.2)



Fig. 13.2: : Redistribution illustration. Excess mass due to using a hybrid divergence D^H instead of the conservative divergence D^C is distributed to neighbor cells.

13.2 Initializing the Geometric Database

In AMReX geometric information is stored in a distributed database class that must be initialized at the start of the calculation. The procedure for this goes as follows:

- Define an implicit function of position which describes the surface of the embedded object. Specifically, the function class must have a public member function that takes a position and returns a negative value if that position is inside the fluid, a positive value in the body, and identically zero at the embedded boundary.

```
Real operator() (const Array<Real, AMREX_SPACEDIM>& p) const;
```

- Make a EB2::GeometryShop object using the implicit function.
- Build an EB2::IndexSpace with the EB2::GeometryShop object and a Geometry object that contains the information about the domain and the mesh.

Here is a simple example of initialize the database for an embedded sphere.

```
Real radius = 0.5;
Array<Real,AMREX_SPACEDIM> center{0., 0., 0.}; //Center of the sphere
bool inside = false; // Is the fluid inside the sphere?
EB2::SphereIF sphere(radius, center, inside);

auto shop = EB2::makeShop(sphere);

Geometry geom(...);
EB2::Build(shop, geom, 0, 0);
```

13.2.1 Implicit Function

In amrex/Src/EB/, there are a number of predefined implicit function classes for basic shapes. One can use these directly or as template for their own classes.

- AllRegularIF: No embedded boundaries at all.
- BoxIF: Box.
- CylinderIF: Cylinder.
- EllipsoidIF: Ellipsoid.
- PlaneIF: Half-space plane.
- SphereIF: Sphere.

AMReX also provides a number of transformation operations to apply to an object.

- makeComplement: Complement of an object. E.g. a sphere with fluid on outside becomes a sphere with fluid inside.
- makeIntersection: Intersection of two or more objects.
- makeUnion: Union of two or more objects.
- Translate: Translates an object.
- scale: Scales an object.
- rotate: Rotates an object.
- lathe: Creates a surface of revolution by rotating a 2D object around an axis.

Here are some examples of using these functions.

```
EB2::SphereIF sphere1(...);
EB2::SphereIF sphere2(...);
EB2::BoxIF box(...);
EB2::CylinderIF cylinder(...);
EB2::PlaneIF plane(...);
```

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```
// union of two spheres
auto twospheres = EB2::makeUnion(sphere1, sphere2);

// intersection of a rotated box, a plane and the union of two spheres
auto box_plane = EB2::makeIntersection(amrex::rotate(box, ...),
                                         plane,
                                         twospheres);

// scale a cylinder by a factor of 2 in x and y directions, and 3 in z-direction.
auto scylinder = EB2::scale(cylinder, {2., 2., 3.});
```

13.2.2 EB2::GeometryShop

Given an implicit function object, say `f`, we can make a `GeometryShop` object with

```
auto shop = EB2::makeShop(f);
```

13.2.3 EB2::IndexSpace

We build `EB2::IndexSpace` with a template function

```
template <typename G>
void EB2::Build (const G& gshop, const Geometry& geom,
                 int required_coarsening_level,
                 int max_coarsening_level,
                 int ngrow = 4);
```

Here the template parameter is a `EB2::GeometryShop`. `Geometry` (see section *RealBox and Geometry*) describes the rectangular problem domain and the mesh on the finest AMR level. Coarse level EB data is generated from coarsening the original fine data. The `int required_coarsening_level` parameter specifies the number of coarsening levels required. This is usually set to $N - 1$, where N is the total number of AMR levels. The `int max_coarsening_levels` parameter specifies the number of coarsening levels AMReX should try to have. This is usually set to a big number, say 20 if multigrid solvers are used. This essentially tells the build to coarsen as much as it can. If there are no multigrid solvers, the parameter should be set to the same as `required_coarsening_level`. It should be noted that coarsening could create multi-valued cells even if the fine level does not have any multi-valued cells. This occurs when the embedded boundary cuts a cell in such a way that there is fluid on multiple sides of the boundary within that cell. Because multi-valued cells are not supported, it will cause a runtime error if the required coarsening level generates multi-valued cells. The optional `int ngrow` parameter specifies the number of ghost cells outside the domain on required levels. For levels coarser than the required level, no EB data are generated for ghost cells outside the domain.

The newly built `EB2::IndexSpace` is pushed on to a stack. Static function `EB2::IndexSpace::top()` returns a `const &` to the new `EB2::IndexSpace` object. We usually only need to build one `EB2::IndexSpace` object. However, if your application needs multiple `EB2::IndexSpace` objects, you can save the pointers for later use. For simplicity, we assume there is only one `EB2::IndexSpace` object for the rest of this chapter.

13.3 EBFArrayBoxFactory

After the EB database is initialized, the next thing we build is `EBFArrayBoxFactory`. This object provides access to the EB database in the format of basic AMReX objects such as `BaseFab`, `FArrayBox`, `FabArray`, and `MultiFab`. We can construct it with

```
EBFArrayBoxFactory (const Geometry& a_geom,
                    const BoxArray& a_ba,
                    const DistributionMapping& a_dm,
                    const Vector<int>& a_ngrow,
                    EBSupport a_support);
```

or

```
std::unique_ptr<EBFArrayBoxFactory>
makeEBFabFactory (const Geometry& a_geom,
                  const BoxArray& a_ba,
                  const DistributionMapping& a_dm,
                  const Vector<int>& a_ngrow,
                  EBSupport a_support);
```

Argument `Vector<int> const& a_ngrow` specifies the number of ghost cells we need for EB data at various `EBSupport` levels, and argument `EBSupport a_support` specifies the level of support needed.

- `EBSupport::basic`: basic flags for cell types
- `EBSupport::volume`: basic plus volume fraction and centroid
- `EBSupport::full`: volume plus area fraction, boundary centroid and face centroid

`EBFArrayBoxFactory` is derived from `FabFactory<FArrayBox>`. `MultiFab` constructors have an optional argument `const FabFactory<FArrayBox>&`. We can use `EBFArrayBoxFactory` to build `MultiFab`s that carry EB data. Member function of `FabArray`

```
const FabFactory<FAB>& Factory () const;
```

can then be used to return a reference to the `EBFArrayBoxFactory` used for building the `MultiFab`. Using `dynamic_cast`, we can test whether a `MultiFab` is built with an `EBFArrayBoxFactory`.

```
auto factory = dynamic_cast<EBFArrayBoxFactory const*>(&(mf.Factory()));  
if (factory) {  
    // this is EBFArrayBoxFactory  
} else {  
    // regular FabFactory<FArrayBox>  
}
```

13.4 EB Data

Through member functions of `EBFArrayBoxFactory`, we have access to the following data:

```
// see section on EBCellFlagFab  
const FabArray<EBCellFlagFab>& getMultiEBCellFlagFab () const;  
  
// volume fraction  
const MultiFab& getVolFrac () const;  
  
// volume centroid  
const MultiCutFab& getCentroid () const;  
  
// embedded boundary centroid  
const MultiCutFab& getBndryCent () const;
```

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```
// area fractions
Array<const MultiCutFab*, AMREX_SPACEDIM> getAreaFrac () const;

// face centroid
Array<const MultiCutFab*, AMREX_SPACEDIM> getFaceCent () const;
```

Volume fraction is in a single-component MultiFab, and it is zero for covered cells, one for regular cells, and in between for cut cells. Centroid is in a MultiCutFab with AMREX_SPACEDIM components with each component of the data is in the range of $[-0.5, 0.5]$. The centroid is based on each cell's local coordinates with respect to the embedded boundary. A MultiCutFab is very similar to a MultiFab. Its data can be accessed with subscript operator

```
const CutFab& operator[] (const MFIter& mfi) const;
```

Here CutFab is derived from FArrayBox and can be passed to Fortran just like FArrayBox. The difference between MultiCutFab and MultiFab is that to save memory MultiCutFab only has data on boxes that contain cut cells. It is an error to call `operator[]` if that box does not have cut cells. Thus the call must be in a `if` test block (see section [EBCellFlagFab](#)). Boundary centroid is also a MultiCutFab with AMREX_SPACEDIM components, and it uses each cell's local coordinates. Area fractions and face centroids are returned in Array of MultiCutFab pointers. For each direction, area fraction is for the face of that direction. As for face centroids, there are two components for each direction and the ordering is always the same as the original ordering of the coordinates. For example, for y face, the component 0 is for x coordinate and 1 for z . The coordinates are in each face's local frame normalized to the range of $[-0.5, 0.5]$.

13.4.1 EBCellFlagFab

EBCellFlagFab contains information on cell types. We can use it to determine if a box contains cut cells.

```
auto const& flags = factory->getMultiEBCellFlagFab();
MultiCutFab const& centroid = factory->getCentroid();

for (MFIter mfi ...) {
    const Box& bx = mfi.tilebox();
    FabType t = flags[mfi].getType(bx);
    if (FabType::regular == t) {
        // This box is regular
    } else if (FabType::covered == t) {
        // This box is covered
    } else if (FabType::singlevalued == t) {
        // This box has cut cells
        // Getting cutfab is safe
        const auto& centroid_fab = centroid[mfi];
    }
}
```

EBCellFlagFab is derived from BaseFab. Its data are stored in an array of 32-bit integers, and can be used in C++ or passed to Fortran just like an IArrayBox (section [BaseFab, FArrayBox and IArrayBox](#)). AMReX provides a Fortran module called `amrex_ebccellflag_module`. This module contains procedures for testing cell types and getting neighbor information. For example

```
use amrex_ebccellflag_module, only : is_regular_cell, is_single_valued_cell, is_
    ↪covered_cell

integer, intent(in) :: flags(...)
```

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```

integer :: i,j,k

do k = ...
do j = ...
do i = ...
  if (is_covered_cell(flags(i,j,k))) then
    ! this is a completely covered cell
  else if (is_regular_cell(flags(i,j,k))) then
    ! this is a regular cell
  else if (is_single_valued_cell(flags(i,j,k))) then
    ! this is a cut cell
  end if
end do
end do
end do

```

13.5 Linear Solvers

Linear solvers for the canonical form (equation (10.1)) have been discussed in chapter [Linear Solvers](#). Currently, AMReX supports cell-centered solver with homogeneous Neumann boundary condition on the EB. A cell-centered solver with Dirichlet boundary condition on the EB and a nodal solver are under development.

To use cell-centered solver for EB, one builds linear operator MLEBABCelLap with EBFArrayBoxFactory.

```

MLEBABCelLap (const Vector<Geometry>& a_geom,
                const Vector<BoxArray>& a_grids,
                const Vector<DistributionMapping>& a_dmap,
                const LPInfo& a_info,
                const Vector<EBFArrayBoxFactory const*>& a_factory);

```

The usage of this EB specified class is essentially the same as MLABecLaplacian.

13.6 Tutorials

amrex/Tutorials/EB/CNS is an AMR code for solving compressible Navier-Stokes equations with the embedded boundary approach.

CHAPTER
FOURTEEN

GPU

In this chapter, we will present the GPU support in AMReX. Currently AMReX only supports Nvidia GPUs. Internally, it uses CUDA C++, but the users can use CUDA Fortran and/or OpenACC. A recent version of CUDA (e.g., ≥ 9) is required, and the device must have compute capability ≥ 6 .

CUDA version 9.2.x is incompatible with AMReX's GPU support due to issues with required compiler flags.

For complete details of CUDA, CUDA Fortran and OpenACC languages, see their respective documentations.

A number of tutorials can be found at [Tutorials/GPU/](#).

14.1 Overview of AMReX GPU Strategy

AMReX's GPU strategy focuses on providing performant GPU support with minimal changes and maximum flexibility. This allows application teams to get running on GPUs quickly while allowing long term performance tuning and programming model selection. AMReX uses CUDA for GPUs, but application teams can use CUDA, CUDA Fortran, OpenACC or OpenMP in their individual codes.

When running AMReX on a CPU system, the parallelization strategy is a combination of MPI and OpenMP using tiling, as detailed in [MFIter with Tiling](#). However, cache blocking and data locality are not the primary considerations when writing optimal code on GPUs. Instead, efficient use of the GPU's resources is the primary concern. Improving resource efficiency allows a larger percentage of GPU threads to work simultaneously, increasing effective parallelism and decreasing the time to solution.

The GPU strategy that has shown to best match AMReX's mesh and particle implementations is MPI+OpenMP for CPUs and MPI+CUDA for GPUs: (MPI+OpenMP) + (MPI+CUDA). Presented here is an overview of important features of AMReX's GPU strategy. Additional information that is required for creating GPU applications is detailed throughout the rest of this chapter:

- To ensure data consistency, each MPI rank offloads its work to a single GPU. This ensures each kernel works on a GPU where the associated data is consistently located and minimizes communication between GPUs. ($\text{MPI ranks} == \text{Number of GPUs}$)
- Calculations that can be offloaded efficiently to GPUs use CUDA threads to parallelize over a valid box at a time. This is done by using a lot of CUDA threads that only work on a few cells each. This work distribution is illustrated in [Table 14.1](#). (Note: OpenMP is currently incompatible with AMReX builds using CUDA. This feature is under development, although most applications will have no need for this feature when initially converting to GPUs.)

Table 14.1: Comparison of OpenMP and CUDA work distribution. Pictures provided by Mike Zingale and the CASTRO team.

| | |
|---|---|
| | |
| <p>OpenMP tiled box. OpenMP threads break down the valid box into two large boxes (blue and orange). The lo and hi of one tiled box are marked.</p> | <p>CUDA threaded box. Each CUDA thread works on a few cells of the valid box. This example uses one cell per thread, each thread using a box with $\text{lo} = \text{hi}$.</p> |

- C++ macros and CUDA extended lambdas are used to provide performance portability while making the code as understandable as possible to science-focused code teams.
- AMReX’s data movement plan is to initialize mesh and particle data structures, move them to the GPU and leave them in GPU memory space as much as possible. This strategy lends itself to AMReX applications readily; the mesh and particle data should be able to stay on the GPU except when performing redistribution and I/O operations. Application teams should strive to this data management strategy as much as possible to achieve good GPU performance.
- AMReX utilizes CUDA managed memory to automatically handle memory movement for mesh and particle data. Simple data structures, such as `IntVects` can be passed by value and temporaries, such as `FArrayBoxes`, have specialized AMReX classes to handle the data movement for the user. Tests have shown CUDA managed memory to be efficient and reliable, especially when applications remove any unnecessary data accesses.
- AMReX’s GPU strategy is focused on launching GPU kernels inside `MFIter` loops. By performing GPU work within `MFIter` loops, GPU work is isolated to independent data sets on simple AMReX data objects, providing consistency and safety that matches AMReX’s coding methodology.
- AMReX further parallelizes GPU applications by utilizing CUDA streams. A CUDA stream is a list of GPU kernel launches that is ran on the GPU sequentially. Kernel launches placed in different CUDA streams can be ran simultaneously on the GPU, given enough computing resources are available. AMReX places each iteration of `MFIter` loops on separate streams, allowing each independent iteration to be ran simultaneously and maximize available GPU resources.

The AMReX implementation of CUDA streams is illustrated in Fig. 14.1. The CPU runs the first iteration of the `MFIter` loop (blue), which contains three GPU kernels. The kernels begin immediately in GPU Stream 1 and run in the same order they were added. The second (red) and third (green) iterations are similarly launched in Streams 2 and 3. The fourth (orange) and fifth (purple) iterations require more GPU resources than remain, so they have to wait until resources are freed before beginning. Meanwhile, after all the loop iterations are launched, the CPU reaches a synchronize in the `MFIter`’s destructor and waits for all GPU launches to complete before continuing.

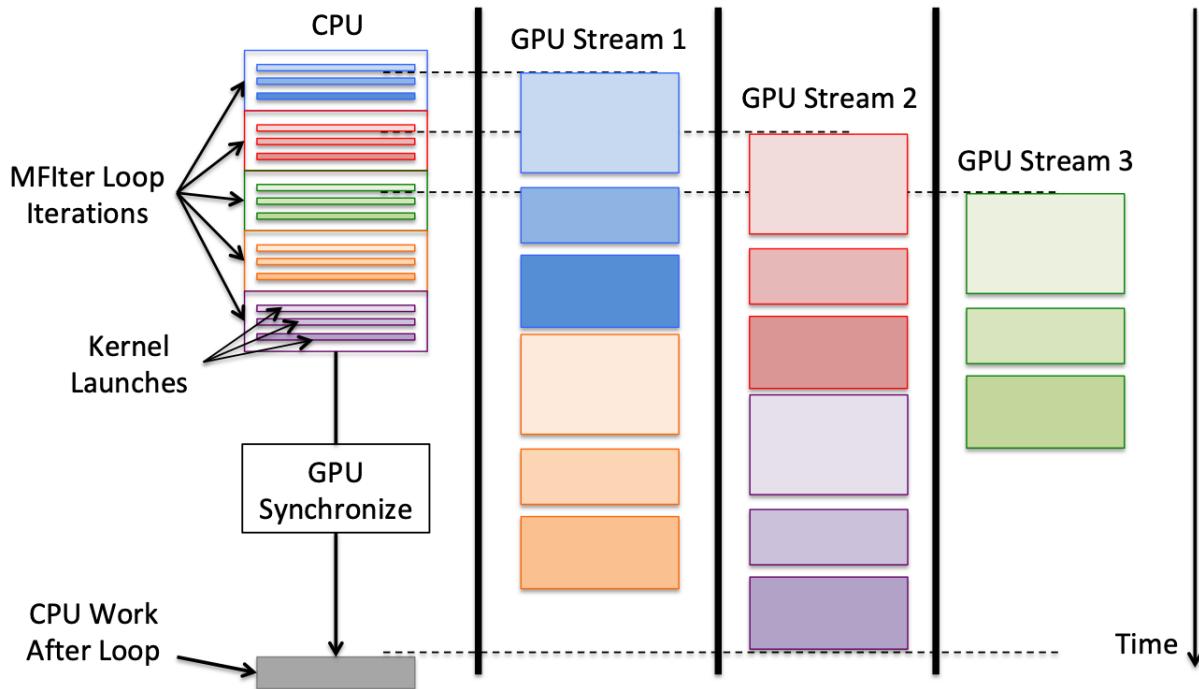


Fig. 14.1: Timeline illustration of GPU streams. Illustrates the case of an MFilter loop of five iterations with three GPU kernels each being ran with three GPU streams.

14.2 Building GPU Support

14.2.1 Building with GNU Make

To build AMReX with GPU support, add `USE_CUDA=TRUE` to the `GNUmakefile` or as a command line argument. AMReX does not require OpenACC or CUDA Fortran, but application codes can use them if they are supported by the compiler. For OpenACC support, add `USE_ACC=TRUE`. PGI, Cray and GNU compilers support OpenACC. Thus, for OpenACC, you must use `COMP=pgi`, `COMP=cray` or `COMP.gnu`. Only IBM and PGI support CUDA Fortran, which is also built when `USE_CUDA=TRUE`. OpenMP is currently not supported with CUDA.

Compiling AMReX with CUDA requires compiling the code through NVIDIA's CUDA compiler driver in addition to the standard compiler. This driver is called `nvcc` and it requires a host compiler to work through. The default host compiler for NVCC is `GCC` even if `COMP` is set to a different compiler. One can change this by setting `NVCC_HOST_COMP`. For example, `COMP=pgi` alone will compile C/C++ codes with NVCC/GCC and Fortran codes with PGI, and link with PGI. Using `COMP=pgi` and `NVCC_HOST_COMP=pgi` will compile C/C++ codes with PGI and NVCC/PGI.

You can use `Tutorials/Basic/HelloWorld_C` to test your programming environment. Building with:

```
make COMP=gnu USE_CUDA=TRUE
```

should produce an executable named `main3d.gnu.DEBUG.CUDA.ex`. You can run it and that will generate results like:

```
$ ./main3d.gnu.DEBUG.CUDA.ex
CUDA initialized with 1 GPU
AMReX (18.12-95-gf265b537f479-dirty) initialized
```

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```
Hello world from AMReX version 18.12-95-gf265b537f479-dirty
[The      Arena] space (kilobyte): 8192
[The Device Arena] space (kilobyte): 8192
[The Managed Arena] space (kilobyte): 8192
[The Pinned Arena] space (kilobyte): 8192
AMReX (18.12-95-gf265b537f479-dirty) finalized
```

14.2.2 Building with CMake

CMake is currently unavailable when building with GPUs.

14.3 Gpu Namespace and Macros

Most GPU related classes and functions are in namespace `Gpu`, which is inside namespace `amrex`. For example, the GPU configuration class `Device` can be referenced to at `amrex::Gpu::Device`. Other important objects in the `Gpu` namespace include `Gpu::AsyncFab`.

For portability, AMReX defines some macros for CUDA function qualifiers and they should be preferred to allow execution with `USE_CUDA=FALSE`. These include:

```
#define AMREX_GPU_HOST      __host__
#define AMREX_GPU_DEVICE     __device__
#define AMREX_GPU_GLOBAL     __global__
#define AMREX_GPU_HOST_DEVICE __host__ __device__
```

Note that when AMReX is not built with CUDA, these macros expand to empty space.

When AMReX is compiled with `USE_CUDA=TRUE`, the preprocessor macros `AMREX_USE_CUDA` and `AMREX_USE_GPU` are defined for conditional programming. For PGI and IBM compilers, `AMREX_USE_CUDA_FORTRAN` is also defined, as well as `-DAMREX_CUDA_FORT_GLOBAL='attributes(global)'`, `-DAMREX_CUDA_FORT_DEVICE='attributes(device)'`, and `-DAMREX_CUDA_FORT_HOST='attributes(host)'` so that CUDA Fortran functions can be properly labelled. When AMReX is compiled with `USE_ACC=TRUE`, `AMREX_USE_ACC` is defined.

In addition to AMReX's preprocessor macros, CUDA provides the `__CUDA_ARCH__` macro which is only defined when in device code. `__CUDA_ARCH__` should be used when a `__host__ __device__` function requires separate code for the CPU and GPU implementations.

14.4 Memory Allocation

To provide portability and improve memory allocation performance, AMReX provides a number of memory pools. When compiled without CUDA, all Arenas implement standard `new` and `delete` operators. Without CUDA, the Arenas each allocate with a specific type of GPU memory:

Table 14.2: Memory Arenas

| Arena | Memory Type |
|---------------------|----------------|
| The_Arena() | unified memory |
| The_Device_Arena() | device memory |
| The_Managed_Arena() | unified memory |
| The_Pinned_Arena() | pinned memory |

The Arena object returned by these calls provides access to two functions:

```
void* alloc (std::size_t sz);
void free (void* p);
```

The_Arena() is used for memory allocation of data in BaseFab. Therefore the data in a MultiFab is placed in unified memory and is accessible from both CPU host and GPU device. This allows application codes to develop their GPU capability gradually. The_Managed_Arena() is a separate pool of unified memory, that is distinguished from The_Arena() for performance reasons. If you want to print out the current memory usage of the Arenas, you can call amrex::Arena::PrintUsage().

14.5 GPU Safe Classes and Functions

AMReX GPU work takes place inside of MFIter and particle loops. Therefore, there are two ways classes and functions have been modified to interact with the GPU:

1. A small number of functions used within these loops are labelled using AMREX_GPU_DEVICE and can be called on the device. This includes member functions, such as IntVect::type(), as well as non-member functions, such as amrex::min and amrex::max. In specialized cases, classes are labeled such that the object can be constructed, destructed and its functions can be implemented on the device, including IntVect.
2. Functions that contain MFIter or particle loops have been rewritten to contain device launches. For example, the FillBoundary function cannot be called from device code, but calling it from CPU will launch GPU kernels if AMReX is compiled with GPU support.

Most functions and objects have not been given a device version due to CUDA restrictions and to ensure applications maintain an internally consistent GPU strategy.

In this section, we discuss some examples of AMReX device classes and functions that are important for programming GPUs.

14.5.1 GpuArray

`std::array` is used throughout AMReX, however its functions are not defined in device code. GpuArray is AMReX's built-in alternative. It uses a C array that can be passed to the device by value and has device functions for the [] operator, size() and data() that returns a pointer to the C array. GpuArray can be used whenever a fixed array of data needs to be passed to the GPU.

Additional functions have been created to return GpuArray instead of `std::array`, including `Box::CellSizeArray()`, `Box::InvCellSizeArray()` and `Box::length3d()`.

14.5.2 ManagedVector

AMReX also provides a dynamic memory allocation object for GPU managed memory: `Gpu::ManagedVector`. This class behaves identically to an `amrex::Vector`, (see [Vector and Array](#)), except the vector's allocator has been

changed to allocate and deallocate its data in CUDA managed memory whenever USE_CUDA=TRUE.

While the data is managed and available on GPUs, the member functions of `Gpu::ManagedVector` are not. To use the data on the GPU, it is necessary to pass the underlying data pointer to the GPU. The managed data pointer can be accessed using the `data()` member function.

Be aware: resizing of dynamically allocated memory on the GPU is unsupported. All resizing of the vector should be done on the CPU, in a manner that avoids race conditions with concurrent GPU kernels.

14.5.3 CUDA's Thrust Vectors

CUDA's Thrust library can also be used to manage dynamically sized data sets. However, if Thrust is used directly in AMReX code, it will be unable to compile for cases when USE_CUDA=FALSE. To alleviate this issue, `thrust::host_vector` and `thrust::device_vector` have been wrapped into the AMReX classes `Gpu::HostVector` and `Gpu::DeviceVector`. When USE_CUDA=FALSE, these classes revert to AMReX's `Vector` class. When USE_CUDA=TRUE, these classes become the corresponding Thrust vector.

Just like with Thrust vectors, `HostVector` and `DeviceVector` cannot be directly used on the device. For convenience, the `dataPtr()` member function has been altered to implement `thrust::raw_pointer_cast` and return the raw data pointer which can be used to access the vector's underlying data on the GPU.

It has proven useful to have a version of Thrust's `device_vector` that uses CUDA managed memory. This is provided by `Gpu::ManagedDeviceVector`.

`thrust::copy` is also commonly used in AMReX applications. It can be implemented portably using `Gpu::thrust_copy`.

14.5.4 amrex::min and amrex::max

GPU versions of `std::min` and `std::max` are not provided in CUDA. So, AMReX provides a templated `min` and `max` with host and device versions to allow functionality on GPUs. Invoke the explicitly namespaced `amrex::min(A, B)` or `amrex::max(x, y)` to use the GPU safe implementations.

14.5.5 MultiFab Reductions

AMReX provides functions for performing standard reduction operations on `Multifabs`, including `MultiFab::sum` and `MultiFab::max`. When USE_CUDA=TRUE, these functions automatically implement the corresponding reductions on GPUs in a highly efficient manner.

Function templates `amrex::ReduceSum`, `amrex::ReduceMin` and `amrex::ReduceMax` can be used to implement user-defined reduction functions over `MultiFabs`. These same templates are implemented in the `Multifab` functions, so they can be used as a reference to build a custom reduction. For example, the `Multifab::dot` implementation is reproduced here:

```
Real sm = amrex::ReduceSum(x, y, nghost,
[=] AMREX_GPU_HOST_DEVICE (Box const& bx, FArrayBox const& xfab, FArrayBox const& yfab) -> Real
{
    return xfab.dot(bx,xcomp,yfab,bx,ycomp,numcomp);
};

if (!local) ParallelAllReduce::Sum(sm, ParallelContext::CommunicatorSub());

return sm;
```

`amrex::ReduceSum` takes two `MultiFab`s, `x` and `y` and returns the sum of the value returned from the given lambda function. In this case, `BaseFab::dot` is returned, yielding a sum of the dot product of each local pair of `BaseFab`s. Finally, `ParallelAllReduce` is used to sum the dot products across all MPI ranks and return the total dot product of the two `MultiFab`s.

To implement a different reduction, replace the code block inside the lambda function with the operation that should be applied, being sure to return the value to be summed, minimized, or maximized. The reduction templates have a few different interfaces to accomodate a variety of reductions. The `amrex::ReduceSum` reduction template has varieties that take either one, two or three `:MultiFab`s. `amrex::ReduceMin` and `amrex::ReduceMax` can take either one or two.

14.5.6 Box, IntVect and IndexType

In AMReX, `Box`, `IntVect` and `IndexType` are classes for representing indices. These classes and most of their member functions, including constructors and destructors, have both host and device versions. They can be used in device code.

14.5.7 Geometry

AMReX's `Geometry` class is not a GPU safe class. However, we often need to use geometric information such as cell size and physical coordinates in GPU kernels. To utilize `Geometry` on the GPUs, the data is copied into a GPU safe class that can be passed by value to GPU kernels. This class is called `GeometryData`, which is created by calling `Geometry::data()`. The accessor functions of `GeometryData` are identical to `Geometry`.

One limitation of this strategy is that `Geometry` cannot not be changed on the device. `GeometryData` holds a disposable copy of the data that does not synchronize with `Geometry` after use. Therefore, only change `Geometry` on the CPU and outside of MFIter loops with GPU kernels to avoid race conditions.

14.5.8 BaseFab, FArrayBox and IArrayBox

`BaseFab<T>`, `IArrayBox` and `FArrayBox` have some GPU support. They cannot be constructed in device code, but a pointer to them can be passed to GPU kernels from CPU code. Many of their member functions can be used in device code as long as they have been allocated in device memory. Some of the device member functions include `view`, `dataPtr`, `box`, `nComp`, and `setVal`.

All `BaseFab<T>` objects in `FabArray<FAB>` are allocated in unified memory, including `MultiFab` and `FArrayBox` which are derived from `BaseFab`. A `BaseFab<T>` object created on the stack in CPU code cannot be used in GPU device code, because the object is in CPU memory. However, a `BaseFab` created with `new` on the heap is GPU safe, because `BaseFab` has its own overloaded `:cpp:operator new` that allocates memory from `The_Arena()`, a managed memory arena. For example,

```
// We are in CPU code

FArrayBox cpu_fab(box,ncomp);
// FArrayBox* p_cpu_fab = &(cpu_fab) cannot be used in GPU device code!

FArrayBox* p_gpu_fab = new FArrayBox(box,ncomp);
// FArrayBox* p_gpu_fab can be used in GPU device code.
```

14.6 Kernel Launch

In this section, how to offload work to the GPU will be demonstrated. In the CUDA C++ and Fortran cases, the kernel is launched with a C++ template global function in AMReX (hidden in an AMReX launch macro), whereas for the OpenACC example, it is done with pragmas in Fortran. More details on the examples can be found in the source codes at `Tutorials/GPU/Launch/`. We also refer the readers to Chapter [Basics](#) for information about basic AMReX classes.

It is also recommended to write your primary floating point operation kernels in C++ using AMReX's `FabView` object syntax. It converts the 1D array into a simple to understand 3D loop structure, similar to Fortran while maintaining performance. The details can be found in [C++ Kernel](#).

14.6.1 Launching a C++ function

The part launching a CUDA C++ kernel is shown below.

```
for (MFIter mfi(mf,TilingIfNotGPU()); mfi.isValid(); ++mfi)
{
    const Box& bx = mfi.tilebox();
    FArrayBox* fab = mf.fabPtr(mfi);
    AMREX_LAUNCH_DEVICE_LAMBDA ( bx, tbx,
    {
        plusone_cudacpp(tbx, *fab);
    });
}
```

The code above works whether it is compiled for GPUs or CPUs. `TilingIfNotGPU()` returns `false` in the GPU case to turn off tiling so that GPU kernels have more compute work to do. When tiling is off, `tilebox()` returns the valid box of the `FArrayBox` for that iteration. The `MultiFab::fabPtr` function takes `MFIter` and returns a managed pointer that can be captured by an extended C++ lambda function the user defined in the `AMREX_LAUNCH_DEVICE_LAMBDA` launch macro.

The launch macro takes three arguments. The first argument is a `Box` specifying the whole region of the kernel. The second argument is the desired name of a `Box` variable that specifies the subregion each thread works on. This subregion `Box` is defined with the specified name inside the macro. The third argument denotes the code block of the lambda function that will be ran in this launch. In this example, a GPU device function, `plusone_cudacpp`, is called and is passed the captured variable `fab`. In CUDA, an extended lambda function can only capture by value, not reference. That's why a pointer must be created to the `FArrayBox`.

14.6.2 Launching a FORTRAN function

We can also call CUDA Fortran device functions in the code block for the launch macro like below.

```
for (MFIter mfi(mf,TilingIfNotGPU()); mfi.isValid(); ++mfi)
{
    const Box& bx = mfi.tilebox();
    FArrayBox* fab = mf.fabPtr(mfi);
    AMREX_LAUNCH_DEVICE_LAMBDA ( bx, tbx,
    {
        plusone_cudafort(BL_TO_FORTRAN_BOX(tbx),
                          BL_TO_FORTRAN_ANYD(*fab));
    });
}
```

Because `Box` and `FArrayBox` are C++ classes not understood by Fortran, we use some helper macros to pass them as Fortran data types (see [Fortran, C and C++ Kernels](#)).

14.6.3 Offloading work using OpenACC pragmas

The tutorial at `Tutorials/GPU/Launch` also shows an example of using OpenACC in Fortran. We call a Fortran function and in that function we use OpenACC to offload work to GPU.

```
for (MFIter mfi(mf,TilingIfNotGPU()); mfi.isValid(); ++mfi)
{
    const Box& bx = mfi.tilebox();
    FArrayBox& fab = mf[mfi];
    plusone_acc(BL_TO_FORTRAN_BOX(bx),
                BL_TO_FORTRAN_ANYD(fab));
}
```

Note that here:`MultiFab::operator[]` is used to get a reference to `FArrayBox` rather than `MultiFab::fabPtr` to get a pointer, as was done in the CUDA examples. Using the reference is optimal for performance when passing pointers to kernels is not required, which includes CPU code sections and OpenACC implementations.

Function `plusone_acc` is a CPU host function. The reference from `operator[]` is a reference to a `FArrayBox` in host memory even though the data pointer inside the object points to unified memory. This managed data pointer is retrieved with `fabPtr`. `BL_TO_FORTRAN_ANYD` expands to the individual components of the `FArrayBox`, including the `Box` defining its indicies, the number of components and the data pointer itself. By passing the `FArrayBox` via its required components, unnecessary data movement is minimized.

The corresponding OpenACC labelled loop in `plusone_acc` is:

```
!dat = pointer to fab's managed data

 !$acc kernels deviceptr(dat)
 do      k = lo(3), hi(3)
   do    j = lo(2), hi(2)
     do i = lo(1), hi(1)
       dat(i,j,k) = dat(i,j,k) + 1.0_amrex_real
     end do
   end do
 end do
 !$acc end kernels
```

Since the data pointer passed to `plusone_acc` points to unified memory, OpenACC is told the data is available on the device by using the `deviceptr` construct.

14.6.4 Launching an generic loop

The previous examples showed how the `AMREX_LAUNCH_DEVICE_LAMBDA` macro can be used to launch threads that work across cells in a `FArrayBox` inside of an `MFIter` loop. However, the macro is also capable of launching for a specified number of iterations that will be split across GPU threads. For example, launching over the number of elements in a vector is an example given in `Tutorials/GPU/Launch` and is reproduced here:

```
{ 
  int size = 100;
  amrex::Gpu::ManagedVector<int> ones(size, 0);
  const auto data = ones.dataPtr();
  AMREX_LAUNCH_DEVICE_LAMBDA(size, iter,
```

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```

    {
        data[iter] = data[iter] + 1;
    });

    Gpu::Device::synchronize();
}

```

A ManagedVector is created that can be worked on from both the CPU and GPU. A copy of the underlying data pointer is created, so it can be captured and passed into the lambda function. The AMREX_LAUNCH_DEVICE_LAMBDA launch macro is used and again it takes three arguments: the size of the vector as a long, a name for the loop iterator and a lambda function to perform on each iteration.

This form of the macro can be used to create any standard, singly incremented loop on a GPU, not just over a vector. This macro can also work on any contiguous subsets of a data set by passing a pointer that points to the beginning of the subset and the size of the subset.

Users must be aware that there is no automatic device synchronize, as these launches do not have to occur inside of an MFIter loop. Add Gpu::Device::synchronize() where necessary to ensure GPU and CPU resources do not alter the same data simultaneously. Lack of automatic GPU stream incrementation is another consequence of being outside an MFIter loop. Users must be aware that if this generic launch is inside a non-MFIter loop all launches will be placed in the default stream, leading to a synchronous implementation of the launches.

14.6.5 Kernel launch details

CUDA kernel calls are asynchronous and they return before the kernel is finished on the GPU. So MFIter finishes its iterations on the CPU before the GPU finishes its work. To guarantee consistency, there is an implicit CUDA device synchronization (a CUDA barrier) in the destructor of MFIter. This ensures that all GPU work inside of an MFIter loop will complete before code outside of the loop is executed.

CUDA supports multiple streams and kernels. Kernels launched in the same stream are executed sequentially, but different streams of kernel launches may be run in parallel. For each iteration of MFIter, AMReX uses a different CUDA stream (up to 16 streams in total) for the kernels in that iteration. This allows each iteration of an MFIter loop to run independently and maximize the use of GPU resources while writing clean, readable MFIter loops.

Launching kernels with the AMREX_LAUNCH_DEVICE_LAMBDA uses the CUDA extended lambda feature. Extended lambdas have some restrictions the user must understand. For example, the function enclosing the extended lambda must not have private or protected access within its parent class, otherwise the code will not compile. This can be fixed by changing the access of the enclosing function to public.

Another pitfall that *must* be considered: if the extended lambda accesses a member of the enclosing class, the lambda function actually captures this pointer by value and accesses variable via this->. If the object is not accessible on GPU, the code will not work as intended. For example,

```

class MyClass {
public:
    Box bx;
    int m; // Unmanaged integer created on the host.
    void f () {
        AMREX_LAUNCH_DEVICE_LAMBDA (bx, tbx,
        {
            printf("m = %d\n", m); // Failed attempt to use m on the GPU.
        });
    }
};

```

The function `f` in the code above will not work unless `MyClass` object is in unified memory. If it is undesirable to put the class into unified memory, a local copy of the information can be created for the lambda to capture. For example:

```
class MyClass {
public:
    Box bx;
    int m;
    void f () {
        int local_m = m; // Local temporary copy of m.
        AMREX_LAUNCH_DEVICE_LAMBDA (bx, tbx,
        {
            printf("m = %d\n", local_m); // Lambda captures local_m by value.
        });
    }
};
```

Finally, AMReX's expected OpenMP strategy for GPUs is to utilize OpenMP in CPU regions to maintain multi-threaded parallelism on work that cannot be offloaded efficiently, while using CUDA independently in GPU regions: (MPI+OpenMP)+(MPI+CUDA). This means OpenMP pragmas need to be maintained when `USE_CUDA=FALSE` and turned off in locations CUDA is implemented when `USE_CUDA=TRUE`.

This can currently be implemented in preparation for an OpenMP strategy and users are highly encouraged to do so now. This prevents having to track down and label the appropriate OpenMP regions in the future and clearly labels for readers that OpenMP and GPUs are not being used at the same time. OpenMP pragmas can be turned off using the conditional pragma and `Gpu::notInLaunchRegion()`, as shown below:

```
#ifdef _OPENMP
#pragma omp parallel if (Gpu::notInLaunchRegion())
#endif
```

14.7 An Example of Migrating to GPU

The nature of GPU programming poses difficulties for a number of common AMReX patterns, such as the one below:

```
// Given MultiFab uin and uout
FArrayBox q;
for (MFIter mfi(uin); mfi.isValid(); ++mfi)
{
    const Box& vbx = mfi.validbox();
    const Box& gbx = amrex::grow(vbx, 1);
    q.resize(gbx);

    // Do some work with uin[mfi] as input and q as output.
    // The output region is gbx;
    f1(gbx, q, uin[mfi]);

    // Then do more work with q as input and uout[mfi] as output.
    // The output region is vbx.
    f2(vbx, uout[mfi], q);
}
```

There are several issues in migrating this code to GPUs that need to be addressed. First, functions `f1` and `f2` have different work regions (`vbx` and `gbx`, respectively) and there are data dependencies between the two (`q`). This makes it difficult to put them into a single GPU kernel, so two separate kernels will be launched, one for each function.

As we have discussed in Section [GPU Safe Classes and Functions](#), all FArrayBoxes in the two MultiFabs, `::cpp::uin` and `uout` are in unified memory and available on the GPUs. But `FArrayBox q` is in host memory. Creating `q` as a managed object using the overloaded `new` operator:

```
FArrayBox* q = new FArrayBox;
```

does not solve the problem completely because GPU kernel calls are asynchronous from CPU's point of view. This creates a race condition: GPU kernels in different iterations of `MFIter` will compete for access to `q`. One possible failure is a segfault when `resize` changes the size of the `q` object when the previous iteration of the loop is still using an old size.

Moving the line into the body of `MFIter` loop will make `q` a variable local to each iteration, but it has a new issue. When do we delete `q`? To the CPU, the resource of `q` should be freed at the end of the scope, otherwise there will be a memory leak. But at the end of the CPU scope, GPU kernels might still need it.

One way to fix this is put the temporary `FArrayBox` objects in a `MultiFab` defined outside the loop. This creates a separate `FArrayBox` for each loop iteration, eliminating the race condition. Another way is to use `Gpu::AsyncFab` designed for this kind of situation. The code below shows how `Gpu::AsyncFab` is used and how this `MFIter` loop can be rewritten for GPUs.

```
for (MFIter mfi(uin); mfi.isValid(); ++mfi)
{
    const Box& vbx = mfi.validbox();                                // f2 work domain
    const Box& gbx = amrex::grow(vbx, 1);                            // f1 work domain
    Gpu::AsyncFab q(gbx);                                            // Local, GPU managed FArrayBox
    FArrayBox const* uinfab = uin.fabPtr();                           // Managed GPU capturable
    FArrayBox      * uoutfab = uout.fabPtr();                          // pointers to Multifab's FABs.

    AMREX_LAUNCH_DEVICE_LAMBDA ( gbx, tbx,                           // f1 GPU launch
    {
        f1(tbx, q.fab(), *uinfab);
    };

    AMREX_LAUNCH_DEVICE_LAMBDA ( vbx, tbx,                           // f2 GPU launch
    {
        f2(tbx, *uoutfab, q.fab());
    });
}                                                               // Implicit GPU barrier after
                                                               // all iters are launched.
```

14.8 Assertions, Error Checking and Synchronization

To help debugging, we often use `amrex::Assert` and `amrex::Abort`. These functions are GPU safe and can be used in GPU kernels. However, implementing these functions requires additional GPU registers, which will reduce overall performance. Therefore, it is preferred to implement such calls in debug mode only by wrapping the calls using `#ifdef AMREX_DEBUG`.

In CPU code, `AMREX_GPU_ERROR_CHECK()` can be called to check the health of previous GPU launches. This call looks up the return message from the most recently completed GPU launch and aborts if it was not successful. Many kernel launch macros as well as the `MFIter` destructor include a call to `AMREX_CPU_ERROR_CHECK()`. This prevents additional launches from being called if a previous launch caused an error and ensures all GPU launches within an `MFIter` loop completed successfully before continuing work.

However, due to asynchronicity, determining the source of the error can be difficult. Even if GPU kernels launched earlier in the code result in a CUDA error, the error may not be output at a nearby call to `AMREX_GPU_ERROR_CHECK()` by the CPU. When tracking down a CUDA launch error,

`Gpu::Device::synchronize()` and `Gpu::Device::streamSynchronize()` can be used to synchronize the device or the CUDA stream, respectively, and track down the specific launch that causes the error.

14.9 Particle Support

AMReX's GPU particle support relies on Thrust, a parallel algorithms library maintained by Nvidia. Thrust provides a GPU-capable vector container that is otherwise similar to the one in the C++ Standard Template Library, along with associated sorting, searching, and prefix summing operations. Combined with Cuda's unified memory, Thrust forms the basis of AMReX's GPU support for particles.

When compiled with `USE_CUDA=TRUE`, AMReX places all its particle data in instances of `thrust::device_vector` that have been configured using a custom memory allocator using `cudaMallocManaged`. This means that the `dataPtr` associated with particle data is managed and can be passed into GPU kernels, similar to the way it would be passed into a Fortran subroutine in typical AMReX CPU code. As with the mesh data, these kernels can be launched with a variety of approaches, including Cuda C / Fortran and OpenACC. An example Fortran particle subroutine offloaded via OpenACC might look like the following:

```

subroutine push_position_boris(np, structs, uxp, uyp, uzp, gaminv, dt)

use em_particle_module, only : particle_t
use amrex_fort_module, only : amrex_real
implicit none

integer,          intent(in), value :: np
type(particle_t), intent(inout)      :: structs(np)
real(amrex_real), intent(in)        :: uxp(np), uyp(np), uzp(np), gaminv(np)
real(amrex_real), intent(in), value :: dt

integer                      :: ip

!$acc parallel deviceptr(structs, uxp, uyp, uzp, gaminv)
!$acc loop gang vector
do ip = 1, np
    structs(ip)%pos(1) = structs(ip)%pos(1) + uxp(ip)*gaminv(ip)*dt
    structs(ip)%pos(2) = structs(ip)%pos(2) + uxp(ip)*gaminv(ip)*dt
    structs(ip)%pos(3) = structs(ip)%pos(3) + uxp(ip)*gaminv(ip)*dt
end do
!$acc end loop
!$acc end parallel

end subroutine push_position_boris

```

Note the use of the `!$acc parallel deviceptr` clause to specify which data has been placed in managed memory. This instructs OpenACC to treat those variables as if they already live on the device, bypassing the usual copies. For a complete example of a particle code that has been ported to GPUs using OpenACC, please see Tutorials/Particles/ElectromagneticPIC.

For portability, we have provided a set of Vector classes that wrap around the Thrust and STL vectors. When `USE_CUDA = FALSE`, these classes reduce to the normal `amrex::Vector`. When `USE_CUDA = TRUE`, they have different meanings. `Cuda::HostVector` is a wrapper around `thrust::host_vector`. `Cuda::DeviceVector` is a wrapper around `thrust::device_vector`, while `Cuda::ManagedDeviceVector` is a `thrust::device_vector` that lives in managed memory. These classes are useful when there are certain stages of an algorithm that will always execute on either the host or the device. For example, the following code generates particles on the CPU and copies them over to the GPU in one batch per tile:

```
for(MFIter mfi = MakeMFIter(lev); mfi.isValid(); ++mfi)
{
    const Box& tile_box = mfi.tilebox();
    Cuda::HostVector<ParticleType> host_particles;

    for (IntVect iv = tile_box.smallEnd(); iv <= tile_box.bigEnd(); tile_box.next(iv))
    {
        < generate some particles... >
    }

    auto& particles = GetParticles(lev);
    auto& particle_tile = particles[std::make_pair(mfi.index(), mfi.
    ↪LocalTileIndex())];
    auto old_size = particle_tile.GetArrayOfStructs().size();
    auto new_size = old_size + host_particles.size();
    particle_tile.resize(new_size);

    Cuda::thrust_copy(host_particles.begin(),
                      host_particles.end(),
                      particle_tile.GetArrayOfStructs().begin() + old_size);
}
```

The following example shows how to use `Cuda::DeviceVector`. Specifically, this code creates temporary device vectors for the particle x, y, and z positions, and then copies from an Array-of-Structs to a Struct-of-Arrays representation, all without copying any particle data off the GPU:

```
Cuda::DeviceVector<Real> xp, yp, zp;

for (WarpXParIter pti(*this, lev); pti.isValid(); ++pti)
{
    pti.GetPosition(xp, yp, zp);

    < use xp, yp, zp... >
}
```

Finally, AMReX's `Redistribute()`, which moves particles back to the proper grids after their positions have changed, has been ported to work on the GPU as well. It cannot be called from device code, but it can be called on particles that reside on the device and it won't trigger any unified memory traffic. As with `Multifab` data, the MPI portion of the particle redistribute is set up to take advantage of the Cuda-aware MPI implementations available on platforms such as ORNL's Summit and Summit-dev.

14.10 Profiling with GPUs

When profiling for GPUs, AMReX recommends `nvprof`, NVIDIA's visual profiler. `nvprof` returns data on how long each kernel launch lasted on the GPU, the number of threads and registers used, the occupancy of the GPU and recommendations for improving the code. For more information on how to use `nvprof`, see NVIDIA's User's Guide as well as the help webpages of your favorite supercomputing facility that uses NVIDIA GPUs.

AMReX's internal profilers currently cannot hook into profiling information on the GPU and an efficient way to time and retrieve that information is being explored. In the meantime, AMReX's timers can be used to report some generic timers that are useful in categorizing an application.

Due to the asynchronous launching of GPU kernels, any AMReX timers inside of asynchronous regions or inside GPU kernels will not measure useful information. However, since the `MFIter` synchronizes when being destroyed, any

timer wrapped around an MFIter loop will yield a consistent timing of the entire set of GPU launches contained within. For example:

```
BL_PROFILE_VAR("MFIter: Init", mfinit);      // Profiling start
for (MFIter mfi(phi_new); mfi.isValid(); ++mfi)
{
    const Box& vbx = mfi.validbox();
    const GeometryData& geomdata = geom.data();
    FArrayBox* phiNew = phi_new.fabPtr(mfi);

    AMREX_LAUNCH_DEVICE_LAMBDA(vbx, tbx,
    {
        init_phi(BL_TO_FORTRAN_BOX(tbx),
                  BL_TO_FORTRAN_ANYD(*phiNew),
                  geomdata.CellSize(), geomdata.ProbLo(), geomdata.ProbHi());
    });
}

BL_PROFILE_STOP(mfinit);                      // Profiling sstop
```

For now, this is the best way to profile GPU codes using TinyProfiler. If you require further profiling detail, use nvprof.

14.11 Performance Tips

Here are some helpful performance tips to keep in mind when working with AMReX for GPUs:

-
-
-

14.12 Limitations

GPU support in AMReX is still under development. There are some known limitations:

- By default, AMReX assumes the MPI library used is GPU aware. The communication buffers given to MPI functions are allocated in device memory.
- OpenMP is currently not compatible with building AMReX with CUDA. USE_CUDA=TRUE and USE_OMP=TRUE will fail to compile.
- CMake is not yet supported for building AMReX GPU support.
- Many multi-level functions in AMReX have not been ported to GPUs.
- Linear solvers have not been ported to GPUs.
- Embedded boundary capability has not been ported to GPUs.
- The Fortran interface of AMReX does not currently have GPU support.

VISUALIZATION

There are several visualization tools that can be used for AMReX plotfiles. The standard tool used within the AMReX-community is Amrvis, a package developed and supported by CCSE that is designed specifically for highly efficient visualization of block-structured hierarchical AMR data. Plotfiles can also be viewed using the VisIt, ParaView, and yt packages. Particle data can be viewed using ParaView.

15.1 Amrvis

Our favorite visualization tool is Amrvis. We heartily encourage you to build the `amrvis1d`, `amrvis2d`, and `amrvis3d` executables, and to try using them to visualize your data. A very useful feature is View/Dataset, which allows you to actually view the numbers in a spreadsheet that is nested to reflect the AMR hierarchy – this can be handy for debugging. You can modify how many levels of data you want to see, whether you want to see the grid boxes or not, what palette you use, etc. Below are some instructions and tips for using Amrvis; you can find additional information in Amrvis/Docs/Amrvis.tex (which you can build into a pdf using pdflatex).

1. Download and build :

```
git clone https://github.com/AMReX-Codes/Amrvis
```

Then cd into Amrvis/, edit the GNUmakefile by setting COMP to the compiler suite you have.

Type `make DIM=1`, `make DIM=2`, or `make DIM=3` to build, resulting in an executable that looks like `amrvis2d...ex`.

If you want to build amrvis with `DIM=3`, you must first download and build volpack:

```
git clone https://ccse.lbl.gov/pub/Downloads/volpack.git
```

Then cd into volpack/ and type make.

Note: Amrvis requires the OSF/Motif libraries and headers. If you don't have these you will need to install the development version of motif through your package manager. `lesstif` gives some functionality and will allow you to build the amrvis executable, but Amrvis may exhibit subtle anomalies.

On most Linux distributions, the motif library is provided by the `openmotif` package, and its header files (like `Xm.h`) are provided by `openmotif-devel`. If those packages are not installed, then use the OS-specific package management tool to install them.

You may then want to create an alias to `amrvis2d`, for example

```
alias amrvis2d /tmp/Amrvis/amrvis2d...ex
```

2. Run the command `cp Amrvis/amrvis.defaults ~/.amrvis.defaults`. Then, in your copy, edit the line containing “palette” line to point to, e.g., “`palette /home/username/Amrvis/Palette`”. The other lines

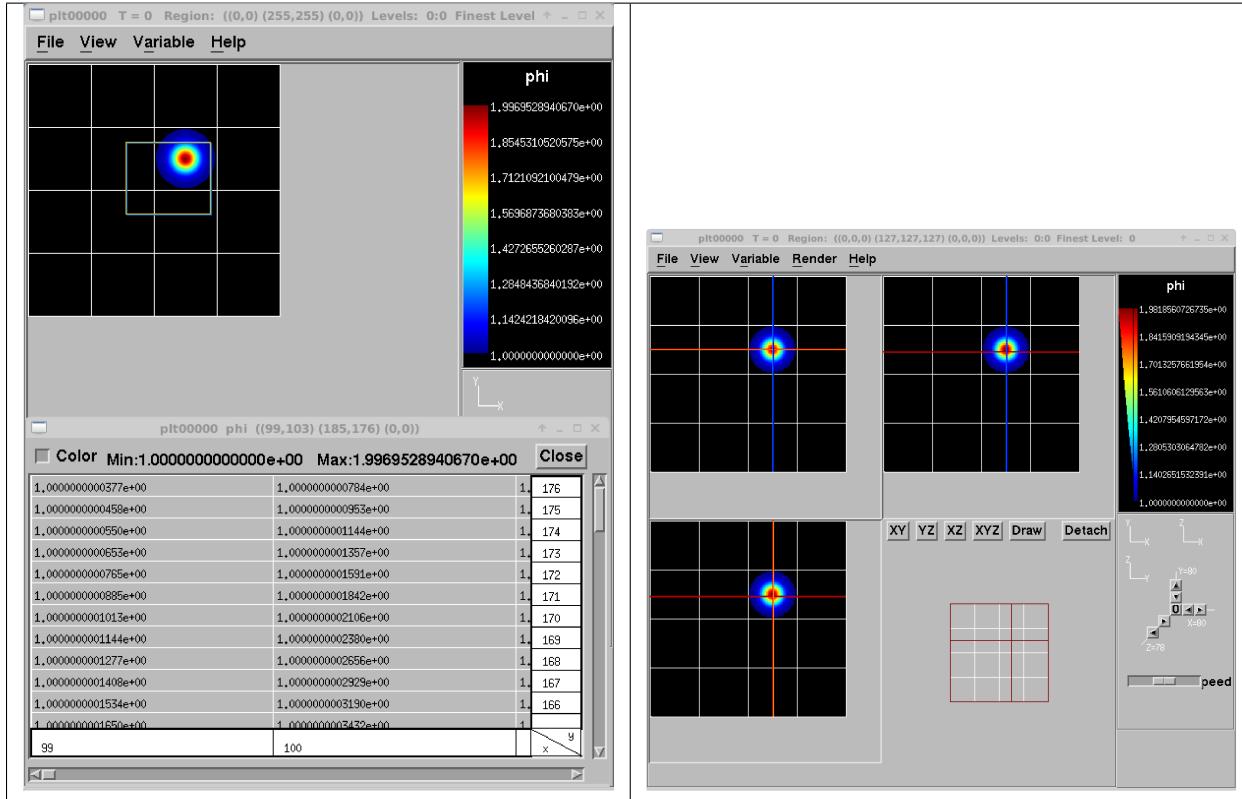
control options such as the initial field to display, the number format, widow size, etc. If there are multiple instances of the same option, the last option takes precedence.

- Generally the plotfiles have the form pltXXXXX (the plt prefix can be changed), where XXXXX is a number corresponding to the timestep the file was output. amrvvis2d <filename> or amrvvis3d <filename> to see a single plotfile, or for 2D data sets, amrvvis2d -a plt*, which will animate the sequence of plotfiles. FArrayBoxes and MultiFabs can also be viewed with the -fab and -mf options. When opening MultiFabs, use the name of the MultiFab's header file amrvvis2d -mf MyMultiFab_H.

You can use the “Variable” menu to change the variable. You can left-click drag a box around a region and click “View” → “Dataset” in order to look at the actual numerical values (see Table 15.1). Or you can simply left click on a point to obtain the numerical value. You can also export the pictures in several different formats under “File/Export”. In 2D you can right and center click to get line-out plots. In 3D you can right and center click to change the planes, and the hold shift+(right or center) click to get line-out plots.

We have created a number of routines to convert AMReX plotfile data other formats (such as matlab), but in order to properly interpret the hierarchical AMR data, each tends to have its own idiosyncrasies. If you would like to display the data in another format, please contact Marc Day (MSDay@lbl.gov) and we will point you to whatever we have that can help.

Table 15.1: 2D and 3D images generated using Amrvvis



15.1.1 Building Amrvvis on macOS

As previously outlined at the end of section [Building with GNU Make](#), it is recommended to build using the [homebrew](#) package manager to install gcc. Furthermore, you will also need x11 and openmotif. These can be installed using homebrew also:

1. brew cask install xquartz

2. brew install openmotif

Note that when the `GNUmakefile` detects a macOS install, it assumes that dependencies are installed in the locations that Homebrew uses. Namely the `/usr/local/` tree for regular dependencies and the `/opt/` tree for X11.

15.2 VisIt

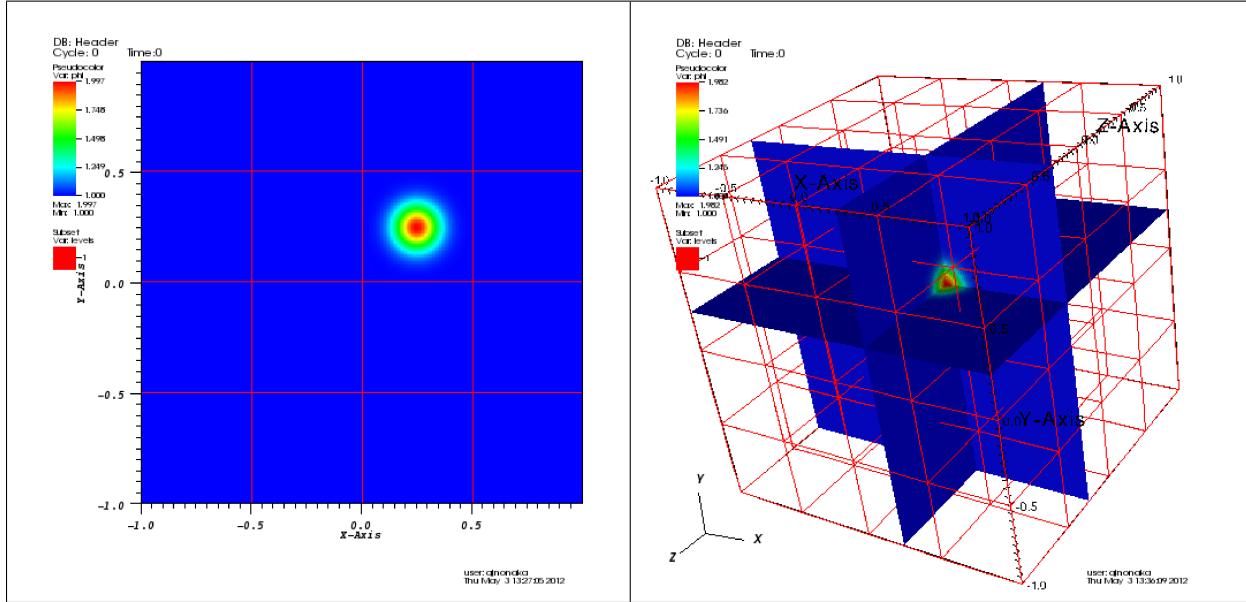
AMReX data can also be visualized by VisIt, an open source visualization and analysis software. To follow along with this example, first build and run the first heat equation tutorial code (see the section on [Example: Heat Equation Solver](#)).

Next, download and install VisIt from <https://wci.llnl.gov/simulation/computer-codes/visit>. To open a single plotfile, run VisIt, then select “File” → “Open file …”, then select the Header file associated with the plotfile of interest (e.g., `plt00000/Header`). Assuming you ran the simulation in 2D, here are instructions for making a simple plot:

- To view the data, select “Add” → “Pseudocolor” → “phi”, and then select “Draw”.
- To view the grid structure (not particularly interesting yet, but when we add AMR it will be), select “→ “subset” → “levels”. Then double-click the text “Subset - levels”, enable the “Wireframe” option, select “Apply”, select “Dismiss”, and then select “Draw”.
- To save the image, select “File” → “Set save options”, then customize the image format to your liking, then click “Save”.

Your image should look similar to the left side of [Table 15.2](#).

Table 15.2: : 2D (left) and 3D (right) images generated using VisIt.



In 3D, you must apply the “Operators” → “Slicing” → “ThreeSlice”, with the “ThreeSlice operator attribute” set to $x=0.25$, $y=0.25$, and $z=0.25$. You can left-click and drag over the image to rotate the image to generate something similar to right side of [Table 15.2](#).

To make a movie, you must first create a text file named `movie.visit` with a list of the Header files for the individual frames. This can most easily be done using the command:

```
~/amrex/Tutorials/Basic/HeatEquation_EX1_C> ls -1 plt*/Header | tee movie.visit
plt0000/Header
plt01000/Header
plt02000/Header
plt03000/Header
plt04000/Header
plt05000/Header
plt06000/Header
plt07000/Header
plt08000/Header
plt09000/Header
plt10000/Header
```

The next step is to run VisIt, select “File” → “Open file …”, then select `movie.visit`. Create an image to your liking and press the “play” button on the VCR-like control panel to preview all the frames. To save the movie, choose “File” → “Save movie …”, and follow the on-screen instructions.

15.3 ParaView

The open source visualization package ParaView v5.5 can be used to view 3D plotfiles, and particle data. Download the package at <https://www.paraview.org/>.

To open a single plotfile (for example, you could run the `HeatEquation_EX1_C` in 3D):

1. Run ParaView v5.5, then select “File” → “Open”.
2. Navigate **into** the plotfile directory, and **manually** type in “Header”. ParaView will ask you about the file type – choose “Boxlib 3D Files”
3. Under the “Cell Arrays” field, select a variable (e.g., “phi”) and click “Apply”.
4. Under “Representation” select “Surface”.
5. Under “Coloring” select the variable you chose above.
6. To add planes, near the top left you will see a cube icon with a green plane slicing through it. If you hover your mouse over it, it will say “Slice”. Click that button.
7. You can play with the Plane Parameters to define a plane of data to view, as shown in Fig. 15.1.

To visualize particle data within plofile directories (for example, you could run the `ShortRangeParticles` example):

1. Run ParaView v5.5, and select then “File” → “Open”. You will see a combined “plt..” group. Click on “+” to expand the group, if you want inspect the files in the group. You can select an individual plotfile directory or select a group of directories to read them a time series, as shown in Fig. 15.2, and click OK.
2. The “Properties” panel in ParaView allows you to specify the “Particle Type”, which defaults to “particles”. Using the “Properties” panel, you can also choose which point arrays to read.
3. Click “Apply” and under “Representation” select “Point Gaussian”.
4. Change the Gaussian Radius if you like. You can scroll through the frames with the VCR-like controls at the top, as shown in Fig. 15.3.

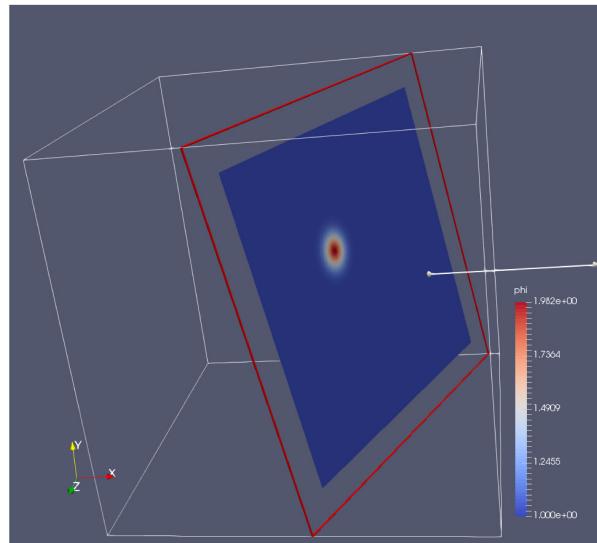


Fig. 15.1: : Plotfile image generated with ParaView

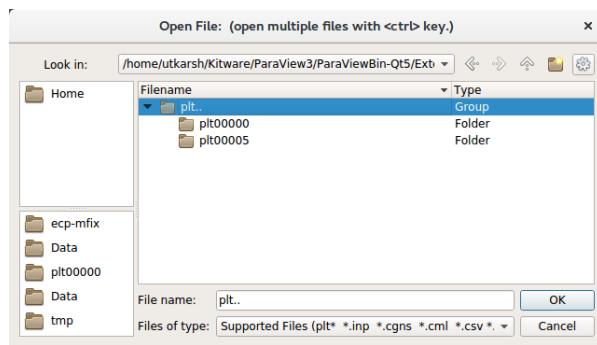


Fig. 15.2: : File dialog in ParaView showing a group of plotfile directories selected

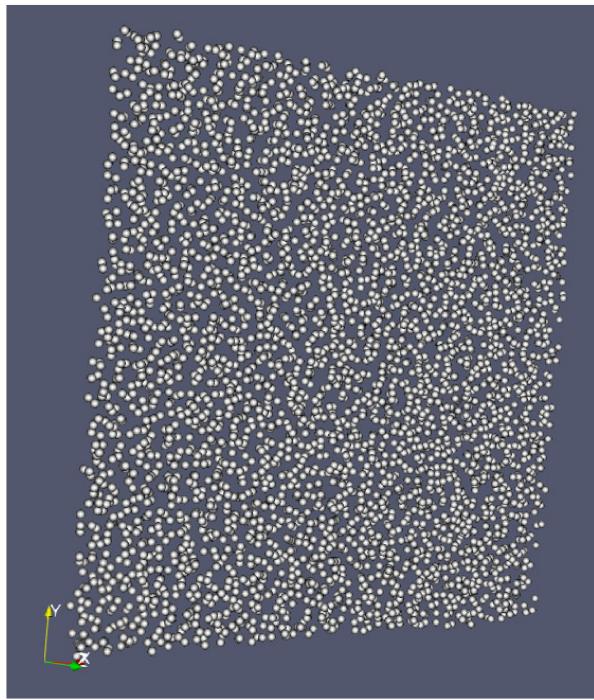


Fig. 15.3: : Particle image generated with ParaView

15.4 yt

yt, an open source Python package available at <http://yt-project.org/>, can be used for analyzing and visualizing mesh and particle data generated by AMReX codes. Some of the AMReX developers are also yt project members. Below we describe how to use yt on both a local workstation, as well as at the NERSC HPC facility for high-throughput visualization of large data sets.

Note - AMReX datasets require yt version 3.4 or greater.

15.4.1 Using on a local workstation

Running yt on a local system generally provides good interactivity, but limited performance. Consequently, this configuration is best when doing exploratory visualization (e.g., experimenting with camera angles, lighting, and color schemes) of small data sets.

To use yt on an AMReX plot file, first start a Jupyter notebook or an IPython kernel, and import the `yt` module:

```
In [1]: import yt
```

```
In [2]: print(yt.__version__)
3.4-dev
```

Next, load a plot file; in this example we use a plot file from the Nyx cosmology application:

```
In [3]: ds = yt.load("plt00401")
yt : [INFO      ] 2017-05-23 10:03:56,182 Parameters: current_time          = 0.
     ↵00605694344696544
yt : [INFO      ] 2017-05-23 10:03:56,182 Parameters: domain_dimensions      = [128
     ↵128 128]
```

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```

yt : [INFO      ] 2017-05-23 10:03:56,182 Parameters: domain_left_edge      = [ 0. ]
  ↵ 0. 0.]
yt : [INFO      ] 2017-05-23 10:03:56,183 Parameters: domain_right_edge     = [ 14.
  ↵24501 14.24501 14.24501]

In [4]: ds.field_list
Out[4]:
[('DM', 'particle_mass'),
 ('DM', 'particle_position_x'),
 ('DM', 'particle_position_y'),
 ('DM', 'particle_position_z'),
 ('DM', 'particle_velocity_x'),
 ('DM', 'particle_velocity_y'),
 ('DM', 'particle_velocity_z'),
 ('all', 'particle_mass'),
 ('all', 'particle_position_x'),
 ('all', 'particle_position_y'),
 ('all', 'particle_position_z'),
 ('all', 'particle_velocity_x'),
 ('all', 'particle_velocity_y'),
 ('all', 'particle_velocity_z'),
 ('boxlib', 'density'),
 ('boxlib', 'particle_mass_density')]

```

From here one can make slice plots, 3-D volume renderings, etc. An example of the slice plot feature is shown below:

```

In [9]: slc = yt.SlicePlot(ds, "z", "density")
yt : [INFO      ] 2017-05-23 10:08:25,358 xlim = 0.000000 14.245010
yt : [INFO      ] 2017-05-23 10:08:25,358 ylim = 0.000000 14.245010
yt : [INFO      ] 2017-05-23 10:08:25,359 xlim = 0.000000 14.245010
yt : [INFO      ] 2017-05-23 10:08:25,359 ylim = 0.000000 14.245010

In [10]: slc.show()

In [11]: slc.save()
yt : [INFO      ] 2017-05-23 10:08:34,021 Saving plot plt00401_Slice_z_density.png
Out[11]: ['plt00401_Slice_z_density.png']

```

The resulting image is Fig. 15.4. One can also make volume renderings with ; an example is show below:

```

In [12]: sc = yt.create_scene(ds, field="density", lens_type="perspective")

In [13]: source = sc[0]

In [14]: source.tfh.set_bounds((1e8, 1e15))

In [15]: source.tfh.set_log(True)

In [16]: source.tfh.grey_opacity = True

In [17]: sc.show()
<Scene Object>:
Sources:
    source_00: <Volume Source>:YTRRegion (plt00401): , center=[ 1.09888770e+25  1.
  ↵09888770e+25  1.09888770e+25] cm, left_edge=[ 0. 0. 0.] cm, right_edge=[ 2.
  ↵19777540e+25  2.19777540e+25  2.19777540e+25] cm transfer_function:None
Camera:

```

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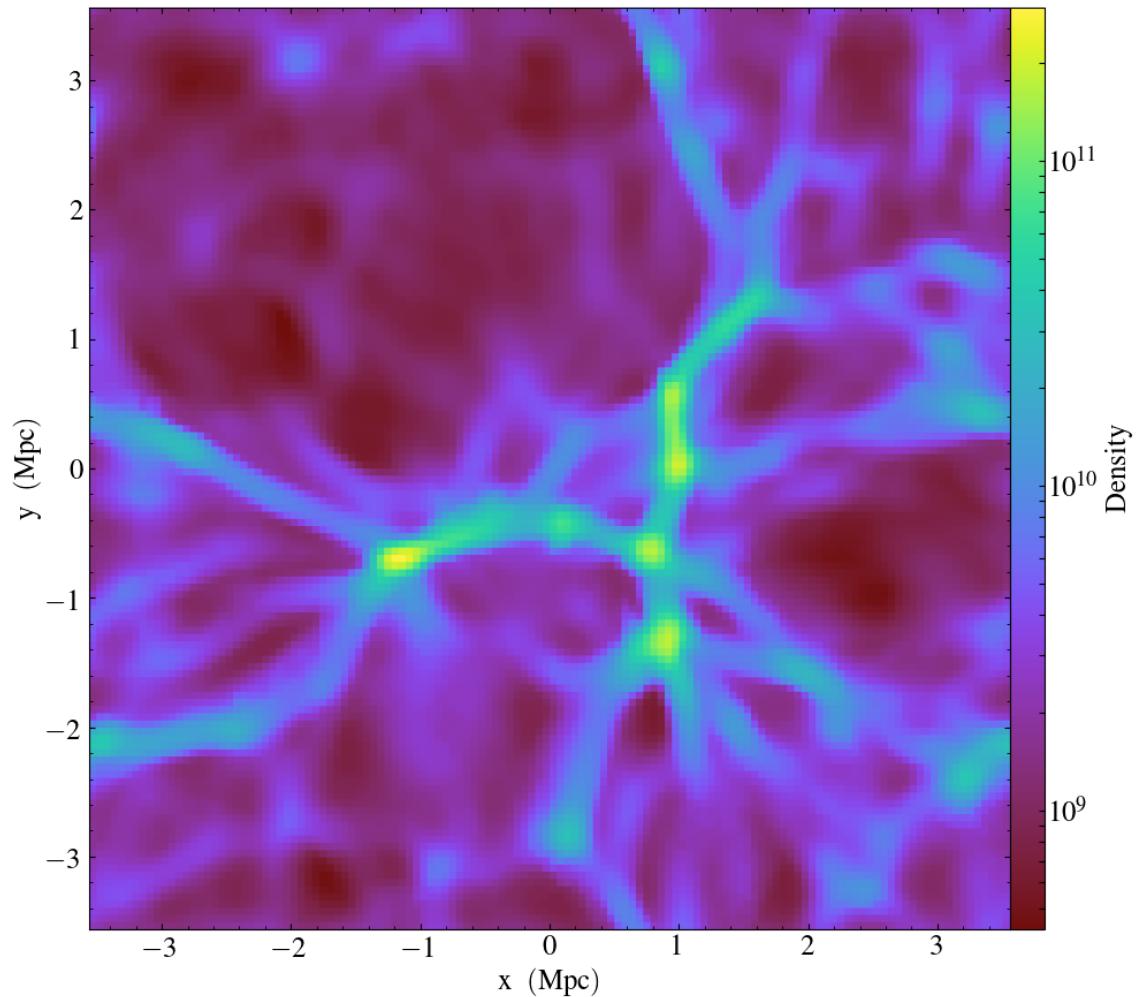


Fig. 15.4: : Slice plot of 128^3 Nyx simulation using yt.

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```

<Camera Object>:
position:[ 14.24501 14.24501 14.24501] code_length
focus:[ 7.122505 7.122505 7.122505] code_length
north_vector:[ 0.81649658 -0.40824829 -0.40824829]
width:[ 21.367515 21.367515 21.367515] code_length
light:None
resolution:(512, 512)
Lens: <Lens Object>:
    lens_type:perspective
    viewpoint:[ 0.95423473 0.95423473 0.95423473] code_length

In [19]: sc.save()
yt : [INFO      ] 2017-05-23 10:15:07,825 Rendering scene (Can take a while).
yt : [INFO      ] 2017-05-23 10:15:07,825 Creating volume
yt : [INFO      ] 2017-05-23 10:15:07,996 Creating transfer function
yt : [INFO      ] 2017-05-23 10:15:07,997 Calculating data bounds. This may take a
      ↵while.
Set the TransferFunctionHelper.bounds to avoid this.
yt : [INFO      ] 2017-05-23 10:15:16,471 Saving render plt00401_Render_density.png

```

The output of this is Fig. 15.5.

15.4.2 Using yt at NERSC (*under development*)

Because yt is Python-based, it is portable and can be used in many software environments. Here we focus on yt's capabilities at NERSC, which provides resources for performing both interactive and batch queue-based visualization and analysis of AMReX data. Coupled with yt's MPI and OpenMP parallelization capabilities, this can enable high-throughput visualization and analysis workflows.

Interactive yt with Jupyter notebooks

Unlike VisIt (see the section on [VisIt](#)), yt has no client-server interface. Such an interface is often crucial when one has large data sets generated on a remote system, but wishes to visualize the data on a local workstation. Both copying the data between the two systems, as well as visualizing the data itself on a workstation, can be prohibitively slow.

Fortunately, NERSC has implemented several resources which allow one to interact with yt remotely, emulating a client-server model. In particular, NERSC now hosts Jupyter notebooks which run IPython kernels on the Cori system; this provides users access to the \$HOME, /project, and \$SCRATCH file systems from a web browser-based Jupyter notebook. ***Please note that Jupyter hosting at NERSC is still under development, and the environment may change without notice.***

NERSC also provides Anaconda Python, which allows users to create their own customizable Python environments. It is recommended to install yt in such an environment. One can do so with the following example:

```

user@cori10:~> module load python/3.5-anaconda
user@cori10:~> conda create -p $HOME/yt-conda numpy
user@cori10:~> source activate $HOME/yt-conda
(/global/homes/u/user/yt-conda/) user@cori10:~> pip install yt

```

More information about Anaconda Python at NERSC is here: <http://www.nersc.gov/users/data-analytics/data-analytics/python/anaconda-python/>.

One can then configure this Anaconda environment to run in a Jupyter notebook hosted on the Cori system. Currently this is available in two places: on <https://ipython.nersc.gov>, and on <https://jupyter-dev.nersc.gov>. The latter likely reflects what the stable, production environment for Jupyter notebooks will look like at NERSC, but it is still

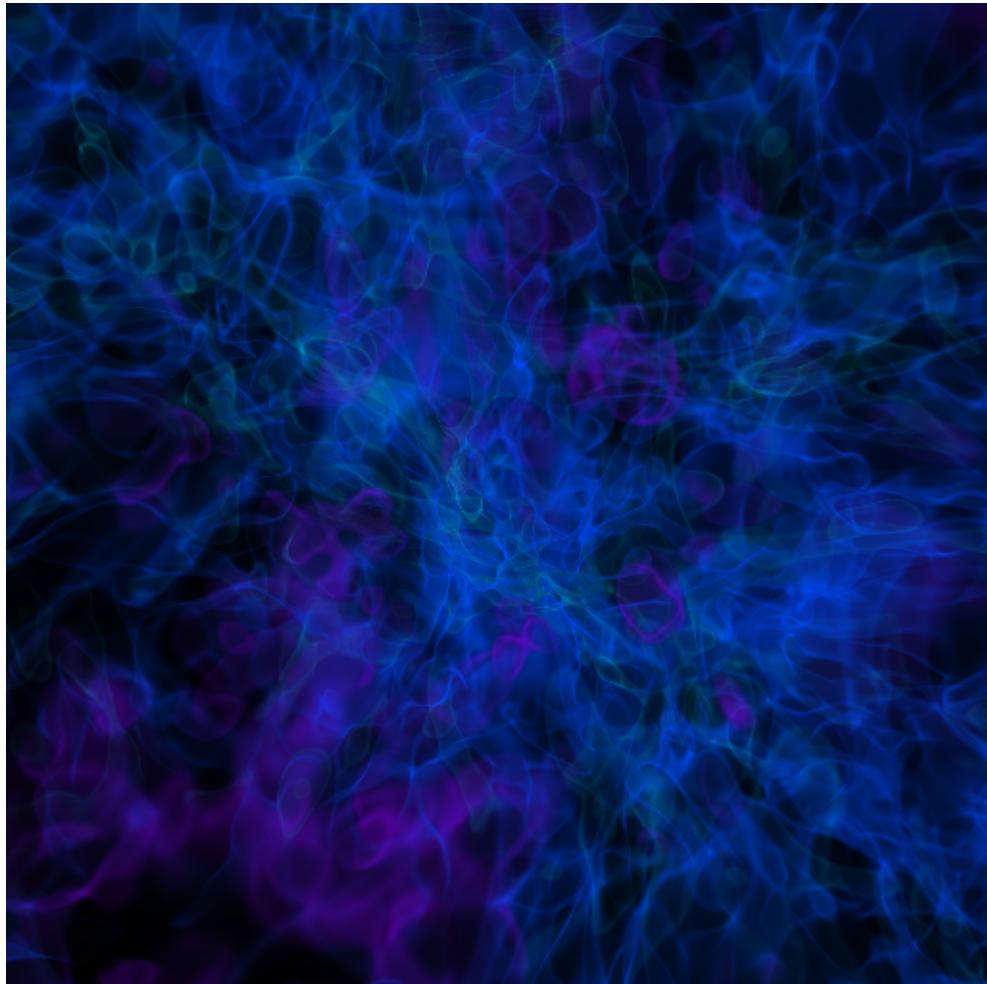


Fig. 15.5: Volume rendering of 128^3 Nyx simulation using yt. This corresponds to the same plot file used to generate the slice plot in Fig. 15.4.

under development and subject to change. To load this custom Python kernel in a Jupyter notebook, follow the instructions at this URL under the “Custom Kernels” heading: <http://www.nersc.gov/users/data-analytics/data-analytics/web-applications-for-data-analytics>. After writing the appropriate `kernel.json` file, the custom kernel will appear as an available Jupyter notebook. Then one can interactively visualize AMReX plot files in the web browser.¹

Parallel

Besides the benefit of no longer needing to move data back and forth between NERSC and one’s local workstation to do visualization and analysis, an additional feature of yt which takes advantage of the computational resources at NERSC is its parallelization capabilities. yt supports both MPI- and OpenMP-based parallelization of various tasks, which are discussed here: http://yt-project.org/doc/analyzing/parallel_computation.html.

Configuring yt for MPI parallelization at NERSC is a more complex task than discussed in the official yt documentation; the command `pip install mpi4py` is not sufficient. Rather, one must compile `mpi4py` from source using the Cray compiler wrappers `cc`, `CC`, and `f77` on Cori. Instructions for compiling `mpi4py` at NERSC are provided here: <http://www.nersc.gov/users/data-analytics/data-analytics/python/anaconda-python/#toc-anchor-3>. After `mpi4py` has been compiled, one can use the regular Python interpreter in the Anaconda environment as normal; when executing yt operations which support MPI parallelization, the multiple MPI processes will spawn automatically.

Although several components of yt support MPI parallelization, a few are particularly useful:

- **Time series analysis.** Often one runs a simulation for many time steps and periodically writes plot files to disk for visualization and post-processing. yt supports parallelization over time series data via the `DatasetSeries` object. yt can iterate over a `DatasetSeries` in parallel, with different MPI processes operating on different elements of the series. This page provides more documentation: http://yt-project.org/doc/analyzing/time_series_analysis.html#time-series-analysis.
- **Volume rendering.** yt implements spatial decomposition among MPI processes for volume rendering procedures, which can be computationally expensive. Note that yt also implements OpenMP parallelization in volume rendering, and so one can execute volume rendering with a hybrid MPI+OpenMP approach. See this URL for more detail: http://yt-project.org/doc/visualizing/volume_rendering.html?highlight=openmp#openmp-parallelization.
- **Generic parallelization over multiple objects.** Sometimes one wishes to loop over a series which is not a `DatasetSeries`, e.g., performing translational or rotational operations on a camera to make a volume rendering in which the field of view moves through the simulation. In this case, one is applying a set of operations on a single object (a single plot file), rather than over a time series of data. For this workflow, yt provides the `parallel_objects()` function. See this URL for more details: http://yt-project.org/doc/analyzing/parallel_computation.html#parallelizing-over-multiple-objects.

An example of MPI parallelization in yt is shown below, where one animates a time series of plot files from an IAMR simulation while revolving the camera such that it completes two full revolutions over the span of the animation:

```
import yt
import glob
import numpy as np

yt.enable_parallelism()

base_dir1 = '/global/cscratch1/sd/user/Nyx_run_p1'
base_dir2 = '/global/cscratch1/sd/user/Nyx_run_p2'
base_dir3 = '/global/cscratch1/sd/user/Nyx_run_p3'
```

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¹ It is convenient to use the magic command `%matplotlib inline` in order to render matplotlib figures in the same browser window as the notebook, as opposed to displaying it as a new window.

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```

glob1 = glob.glob(base_dir1 + '/plt*')
glob2 = glob.glob(base_dir2 + '/plt*')
glob3 = glob.glob(base_dir3 + '/plt*')

files = sorted(glob1 + glob2 + glob3)

ts = yt.DatasetSeries(files, parallel=True)

frame = 0
num_frames = len(ts)
num_revol = 2

slices = np.arange(len(ts))

for i in yt.parallel_objects(slices):
    sc = yt.create_scene(ts[i], lens_type='perspective', field='z_velocity')
    source = sc[0]
    source.tfh.set_bounds((1e-2, 9e+0))
    source.tfh.set_log(False)
    source.tfh.grey_opacity = False

    cam = sc.camera

    cam.rotate(num_revol*(2.0*np.pi)*(i/num_frames),
               rot_center=np.array([0.0, 0.0, 0.0]))

    sc.save(sigma_clip=5.0)

```

When executed on 4 CPUs on a Haswell node of Cori, the output looks like the following:

```

user@nid00009:~/yt_vis/> srun -n 4 -c 2 --cpu_bind=cores python make_yt_
->movie.py
yt : [INFO      ] 2017-05-23 16:51:33,565 Global parallel computation
->enabled: 0 / 4
yt : [INFO      ] 2017-05-23 16:51:33,565 Global parallel computation
->enabled: 2 / 4
yt : [INFO      ] 2017-05-23 16:51:33,566 Global parallel computation
->enabled: 1 / 4
yt : [INFO      ] 2017-05-23 16:51:33,566 Global parallel computation
->enabled: 3 / 4
P003 yt : [INFO      ] 2017-05-23 16:51:33,957 Parameters: current_time
->          = 0.103169376949795
P003 yt : [INFO      ] 2017-05-23 16:51:33,957 Parameters: domain_
->dimensions        = [128 128 128]
P003 yt : [INFO      ] 2017-05-23 16:51:33,957 Parameters: domain_left_
->edge            = [ 0.  0.  0.]
P003 yt : [INFO      ] 2017-05-23 16:51:33,958 Parameters: domain_right_
->edge            = [ 6.28318531  6.28318531  6.28318531]
P000 yt : [INFO      ] 2017-05-23 16:51:33,969 Parameters: current_time
->          = 0.0
P000 yt : [INFO      ] 2017-05-23 16:51:33,969 Parameters: domain_
->dimensions        = [128 128 128]
P002 yt : [INFO      ] 2017-05-23 16:51:33,969 Parameters: current_time
->          = 0.0687808060674485
P000 yt : [INFO      ] 2017-05-23 16:51:33,969 Parameters: domain_left_
->edge            = [ 0.  0.  0.]

```

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```

P002 yt : [INFO      ] 2017-05-23 16:51:33,969 Parameters: domain_
  ↵dimensions      = [128 128 128]
P000 yt : [INFO      ] 2017-05-23 16:51:33,970 Parameters: domain_right_
  ↵edge      = [ 6.28318531  6.28318531  6.28318531]
P002 yt : [INFO      ] 2017-05-23 16:51:33,970 Parameters: domain_left_
  ↵edge      = [ 0.  0.  0.]
P002 yt : [INFO      ] 2017-05-23 16:51:33,970 Parameters: domain_right_
  ↵edge      = [ 6.28318531  6.28318531  6.28318531]
P001 yt : [INFO      ] 2017-05-23 16:51:33,973 Parameters: current_time
  ↵          = 0.0343922351851018
P001 yt : [INFO      ] 2017-05-23 16:51:33,973 Parameters: domain_
  ↵dimensions      = [128 128 128]
P001 yt : [INFO      ] 2017-05-23 16:51:33,974 Parameters: domain_left_
  ↵edge      = [ 0.  0.  0.]
P001 yt : [INFO      ] 2017-05-23 16:51:33,974 Parameters: domain_right_
  ↵edge      = [ 6.28318531  6.28318531  6.28318531]
P000 yt : [INFO      ] 2017-05-23 16:51:34,589 Rendering scene (Can take a
  ↵while).
P000 yt : [INFO      ] 2017-05-23 16:51:34,590 Creating volume
P003 yt : [INFO      ] 2017-05-23 16:51:34,592 Rendering scene (Can take a
  ↵while).
P002 yt : [INFO      ] 2017-05-23 16:51:34,592 Rendering scene (Can take a
  ↵while).
P003 yt : [INFO      ] 2017-05-23 16:51:34,593 Creating volume
P002 yt : [INFO      ] 2017-05-23 16:51:34,593 Creating volume
P001 yt : [INFO      ] 2017-05-23 16:51:34,606 Rendering scene (Can take a
  ↵while).
P001 yt : [INFO      ] 2017-05-23 16:51:34,607 Creating volume

```

Because the `parallel_objects()` function transforms the loop into a data-parallel problem, this procedure strong scales nearly perfectly to an arbitrarily large number of MPI processes, allowing for rapid rendering of large time series of data.

15.5 SENSEI

SENSEI is a light weight framework for in situ data analysis. SENSEI's data model and API provide uniform access to and run time selection of a diverse set of visualization and analysis back ends including VisIt Libsim, ParaView Catalyst, VTK-m, Ascent, ADIOS, Yt, and Python.

15.5.1 System Architecture

The three major architectural components in SENSEI are *data adaptors* which present simulation data in SENSEI's data model, *analysis adaptors* which present the back end data consumers to the simulation, and *bridge code* from which the simulation manages adaptors and periodically pushes data through the system. SENSEI comes equipped with a number of analysis adaptors enabling use of popular analysis and visualization libraries such as VisIt Libsim, ParaView Catalyst, Python, and ADIOS to name a few. AMReX contains SENSEI data adaptors and bridge code making it easy to use in AMReX based simulation codes.

SENSEI provides a *configurable analysis adaptor* which uses an XML file to select and configure one or more back ends at run time. Run time selection of the back end via XML means one user can access Catalyst, another Libsim, yet another Python with no changes to the code. This is depicted in figure Fig. 15.6. On the left side of the figure AMReX produces data, the bridge code pushes the data through the configurable analysis adaptor to the back end that was selected at run time.

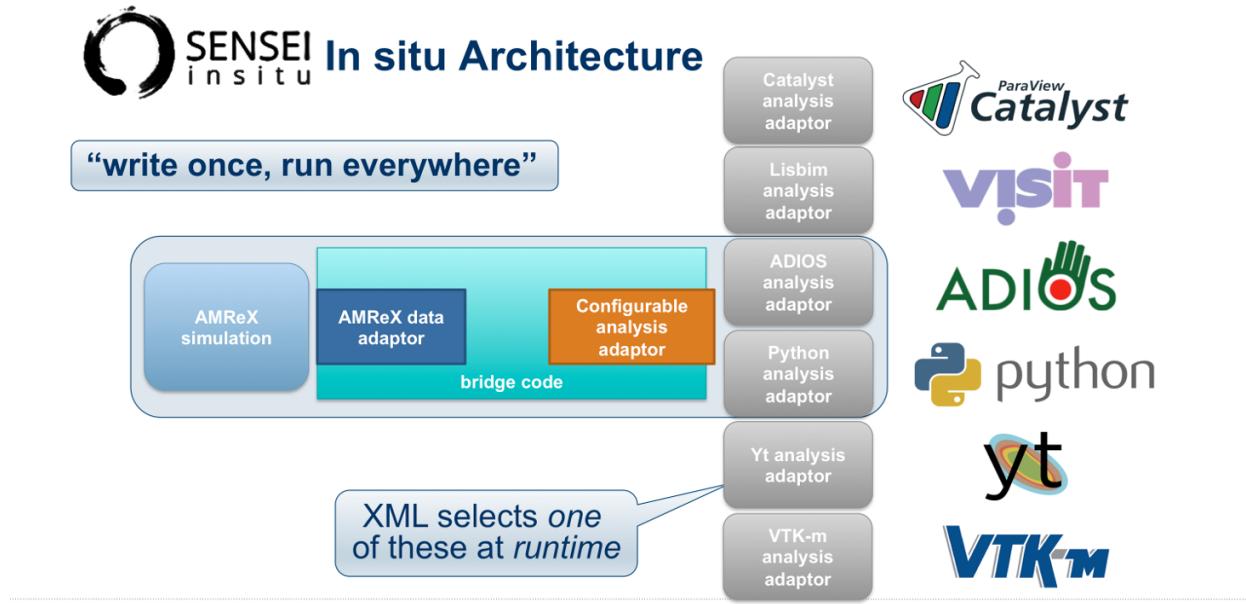


Fig. 15.6: SENSEI's in situ architecture enables use of a diverse of back ends which can be selected at run time via an XML configuration file

15.5.2 AMReX Integration

AMReX codes based on `amrex::Amr` can use SENSEI simply by enabling it in the build and run via ParmParse parameters. AMReX codes based on `amrex::AmrMesh` need to additionally invoke the bridge code in `amrex::AmrMeshInSituBridge`.

15.5.3 Compiling with GNU Make

For codes making use of AMReX's build system add the following variable to the code's main `GNUmakefile`.

```
USE_SENSEI_INSITU = TRUE
```

When set, AMReX's make files will query environment variables for the lists of compiler and linker flags, include directories, and link libraries. These lists can be quite elaborate when using more sophisticated back ends, and are best set automatically using the `sensei_config` command line tool that should be installed with SENSEI. Prior to invoking make use the following command to set these variables:

```
source sensei_config
```

Typically, the `sensei_config` tool is in the users PATH after loading the desired SENSEI module. After configuring the build environment with `sensei_config`, proceed as usual.

```
make -j4 -f GNUmakefile
```

15.5.4 Compiling with CMake

For codes making use of AMReX's CMake based build, one needs to enable SENSEI and point to the CMake configuration installed with SENSEI.

```
cmake -DENABLE_SENSEI=ON -DSENSEI_DIR=<path to install>/lib/cmake ...
```

When CMake generates the make files proceed as usual.

```
make -j4 -f GNUmakefile
```

15.5.5 ParmParse Configuration

Once an AMReX code has been compiled with SENSEI features enabled, it will need to be enabled and configured at runtime. This is done using ParmParse input file. The following 3 ParmParse parameters are used:

```
sensei.enabled = 1
sensei.config = render_iso_catalyst_2d.xml
sensei.frequency = 2
```

`sensei.enabled` turns SENSEI on or off. `sensei.config` points to the SENSEI XML file which selects and configures the desired back end. `sensei.frequency` controls the number of level 0 time steps in between SENSEI processing.

15.5.6 Back-end Selection and Configuration

The back end is selected and configured at run time using the SENSEI XML file. The XML sets parameters specific to SENSEI and to the chosen back end. Many of the back ends have sophisticated configuration mechanisms which SENSEI makes use of. For example the following XML configuration was used on NERSC's Cori with IAMR to render 10 iso surfaces, shown in figure Fig. 15.7, using VisIt Libsim.

```
<sensei>
  <analysis type="libsime" frequency="1" mode="batch"
    visitdir="/usr/common/software/sensei/visit"
    session="rt_sensei_configs/visit_rt_contour_alpha_10.session"
    image-filename="rt_contour_%ts" image-width="1555" image-height="815"
    image-format="png" enabled="1"/>
</sensei>
```

The `session` attribute names a session file that contains VisIt specific runtime configuration. The session file is generated using VisIt GUI on a representative dataset. Usually this data set is generated in a low resolution run of the desired simulation.

The same run and visualization was repeated using ParaView Catalyst, shown in figure Fig. 15.8, by providing the following XML configuration.

```
<sensei>
  <analysis type="catalyst" pipeline="pythonscript"
    filename="rt_sensei_configs/rt_contour.py" enabled="1" />
</sensei>
```

Here the `filename` attribute is used to pass Catalyst a Catalyst specific configuration that was generated using the ParaView GUI on a representative dataset.

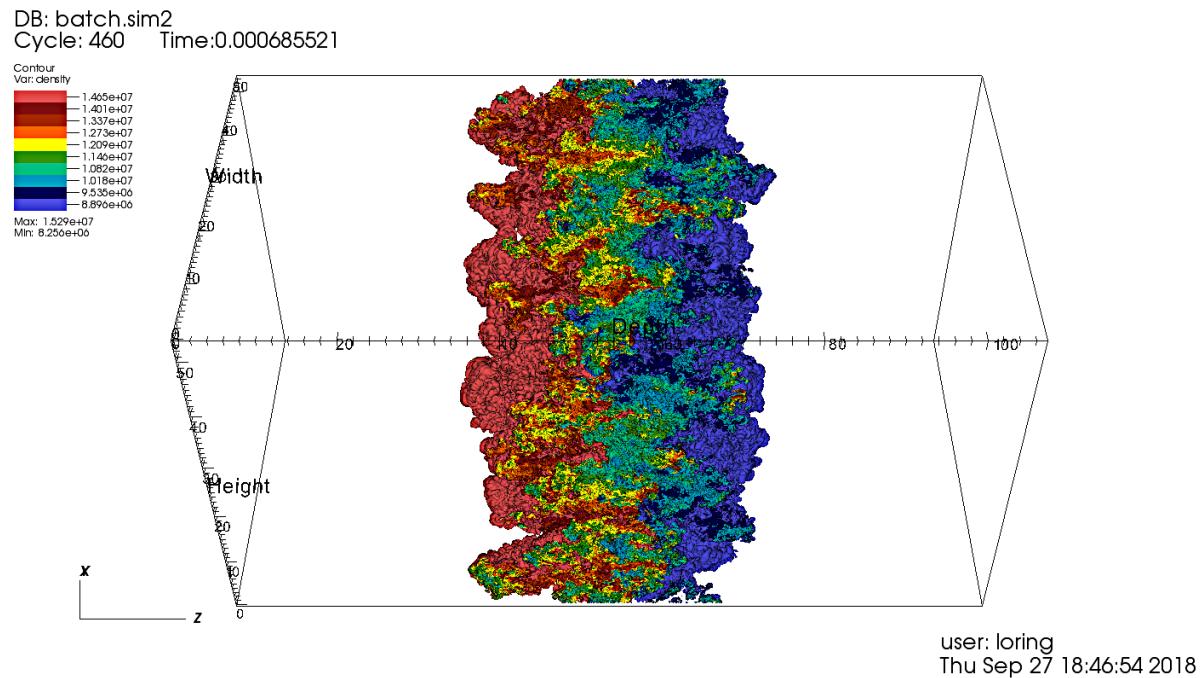


Fig. 15.7: SENSEI-Libsim in situ visualization of a Raleigh-Taylor instability computed by IAMR on NERSC Cori using 2048 cores.

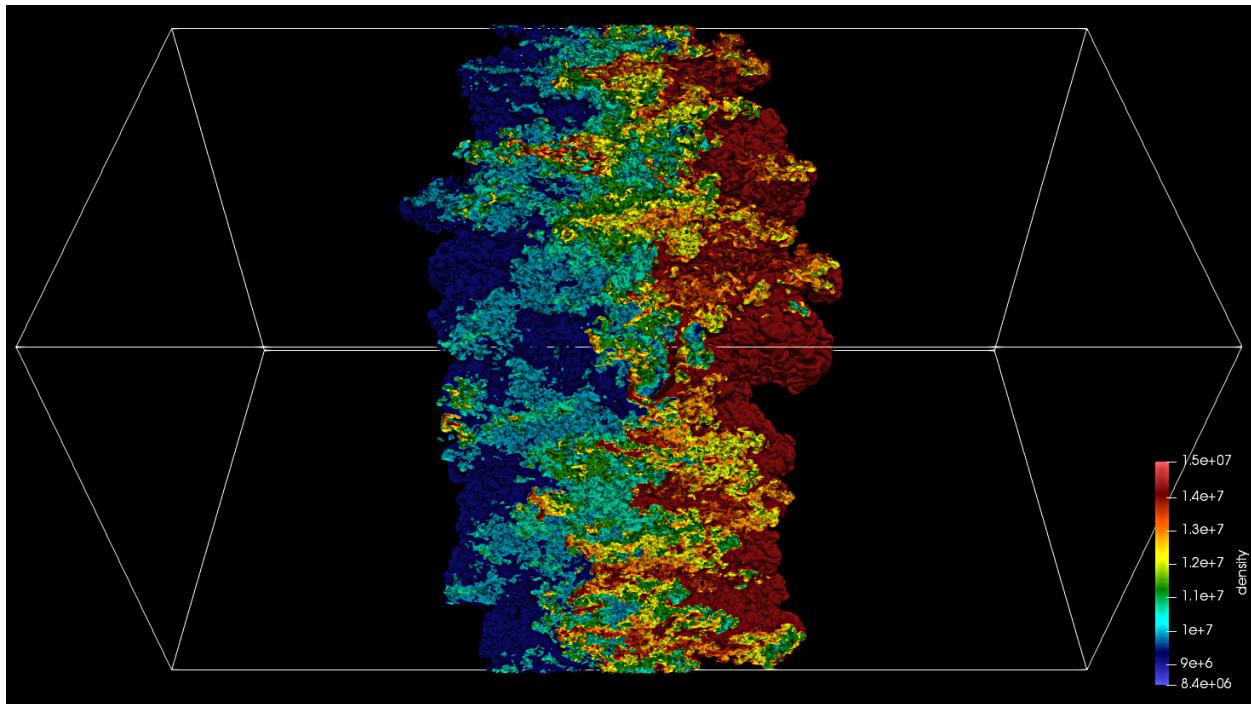


Fig. 15.8: SENSEI-Catalyst in situ visualization of a Raleigh-Taylor instability computed by IAMR on NERSC Cori using 2048 cores.

15.5.7 Obtaining SENSEI

SENSEI is hosted on Kitware’s Gitlab site at <https://gitlab.kitware.com/sensei/sensei>. It’s best to checkout the latest release rather than working on the master branch.

To ease the burden of wrangling back end installs SENSEI provides two platforms with all dependencies pre-installed, a VirtualBox VM, and a NERSC Cori deployment. New users are encouraged to experiment with one of these.

SENSEI VM

The SENSEI VM comes with all of SENSEI’s dependencies and the major back ends such as VisIt and ParaView installed. The VM is the easiest way to test things out. It also can be used to see how installs were done and the environment configured.

NERSC Cori

SENSEI is deployed at NERSC on Cori. The NERSC deployment includes the major back ends such as ParaView Catalyst, VisIt Libsim, and Python.

AmrLevel Tutorial with Catalyst

The following steps show how to run the tutorial with ParaView Catalyst. The simulation will periodically write images during the run.

```
ssh cori.nersc.gov
cd $SCRATCH
git clone https://github.com/AMReX-Codes/amrex.git
cd amrex/Tutorials/Amr/Advection_AmrLevel/Exec/SingleVortex
module use /usr/common/software/sensei/modulefiles
module load sensei/2.1.0-catalyst-shared
source sensei_config
vim GNUmakefile
# USE_SENSEI_INSITU=TRUE
make -j4 -f GNUmakefile
vim inputs
# sensei.enabled=1
# sensei.config=sensei/render_iso_catalyst_2d.xml
salloc -C haswell -N 1 -t 00:30:00 -q debug
cd $SCRATCH/amrex/Tutorials/Amr/Advection_AmrLevel/Exec/SingleVortex
./main2d.gnu.haswell.MPI.ex inputs
```

AmrLevel Tutorial with Libsim

The following steps show how to run the tutorial with VisIt Libsim. The simulation will periodically write images during the run.

```
ssh cori.nersc.gov
cd $SCRATCH
git clone https://github.com/AMReX-Codes/amrex.git
cd amrex/Tutorials/Amr/Advection_AmrLevel/Exec/SingleVortex
module use /usr/common/software/sensei/modulefiles
module load sensei/2.1.0-libsim-shared
```

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```
source sensei_config
vim GNUmakefile
# USE_SENSEI_INSITU=TRUE
make -j4 -f GNUmakefile
vim inputs
# sensei.enabled=1
# sensei.config=sensei/render_iso_libsim_2d.xml
salloc -C haswell -N 1 -t 00:30:00 -q debug
./main2d.gnu.haswell.MPI.ex inputs
```

AMREX-BASED PROFILING TOOLS

AMReX-based application codes can be instrumented using AMReX-specific performance profiling tools that take into account the hierarchical nature of the mesh in most AMReX-based applications. These codes can be instrumented for varying levels of profiling detail.

Here are links to short courses (slides) on how to use the profiling tools. More details can be found in the documentation below.

Lecture 1: [Introduction and TINYPROFILER](#)

Lecture 2: [Introduction to Full Profiling](#)

Lecture 3: [Using ProfVis – GUI Features](#)

Lecture 4: [Batch Options and Advanced Profiling Flags](#)

16.1 Types of Profiling

Currently you have two options for AMReX-specific profiling: *Tiny Profiling* and *Full Profiling*.

16.1.1 Tiny Profiling

To enable “Tiny Profiling”, if using GNU Make then set

```
TINY_PROFILE = TRUE
PROFILE       = FALSE
```

in your GNUMakefile. If using cmake then set the following cmake flags

```
AMREX_ENABLE_TINY_PROFILE = ON
AMREX_ENABLE_BASE_PROFILE = OFF
```

Note that if you set PROFILE = TRUE (or AMREX_ENABLE_BASE_PROFILE = ON) then this will override the TINY_PROFILE flag and tiny profiling will be disabled.

At the end of the run, a summary of exclusive and inclusive function times will be written to stdout. This output includes the minimum and maximum (over processes) time spent in each routine as well as the average and the maximum percentage of total run time. See [Sample Output From Tiny Profile](#) for sample output.

The tiny profiler automatically writes the results to stdout at the end of your code, when `amrex::Finalize()` ; is reached. However, you may want to write partial profiling results to ensure your information is saved when you may fail to converge or if you expect to run out of allocated time. Partial results can be written at user-defined times by inserting the line:

```
BL_PROFILE_TINY_FLUSH();
```

Any timers that have not reached their `BL_PROFILE_VAR_STOP` call or exited their scope and deconstructed will not be included in these partial outputs. (e.g., a properly instrumented `main()` should show a time of zero in all partial outputs.) Therefore, it is recommended to place these flush calls in easily identifiable regions of your code and outside of as many profiling timers as possible, such as immediately before or after writing a checkpoint.

Also, since flush calls will print multiple, similar looking outputs to `stdout`, it is also recommended to wrap any `BL_PROFILE_TINY_FLUSH();` calls in informative `amrex::Print()` lines to ensure accurate identification of each set of timers.

16.1.2 Full Profiling

If you set `PROFILE = TRUE` then a `bl_prof` directory will be written that contains detailed per-task timings for each processor. This will be written in `nfiles` files (where `nfiles` is specified by the user). In addition, an exclusive-only set of function timings will be written to `stdout`.

Trace Profiling

If, in addition to `PROFILE = TRUE`, you set `TRACE_PROFILE = TRUE`, then the profiler keeps track of when each profiled function is called and the `bl_prof` directory will include the function call stack. This is especially useful when core functions, such as `FillBoundary` can be called from many different regions of the code. Part of the trace profiling is the ability to set regions in the code which can be analyzed for profiling information independently from other regions.

Communication Profiling

If, in addition to `PROFILE = TRUE`, you set `COMM_PROFILE = TRUE`, then the `bl_prof` directory will contain additional information about MPI communication (point-to-point timings, data volume, barrier/reduction times, etc.). `TRACE_PROFILE = TRUE` and `COMM_PROFILE = TRUE` can be set together.

The AMReX-specific profiling tools are currently under development and this documentation will reflect the latest status in the development branch.

16.2 Instrumenting C++ Code

You must at least instrument `main()`, i.e

```
int main(...)  
{  
    amrex::Initialize(argc,argv);  
    BL_PROFILE_VAR("main()",pmain);  
  
    ...  
  
    BL_PROFILE_VAR_STOP(pmain);  
    amrex::Finalize();  
}
```

You can then instrument any of your functions

```
void YourClass::YourFunction()
{
    BL_PROFILE_VAR("YourClass::YourFunction()", object_name); // this name can be any
    →string

    // your function code
}
```

Note that you do not need to put BL_PROFILE_VAR_STOP because the profiler will go out of scope at the end of the function.

For other timers within an already instrumented function, add:

```
BL_PROFILE_VAR("Flaten::FORT_FLATENX()", anyname); // add this before
    FORT_FLATENX(arg1, arg2);
BL_PROFILE_VAR_STOP(anyname); // add this after, using the same name
```

if you want to use the same name within the same scope, you can use:

```
BL_PROFILE_VAR("MyFuncs()", myfuncs); // the first one
    MyFunc_0(arg);
BL_PROFILE_VAR_STOP(myfuncs);
...
BL_PROFILE_VAR_START(myfuncs);
    MyFunc_1(arg);
BL_PROFILE_VAR_STOP(myfuncs);
```

or create a profiling variable without starting, then start/stop:

```
BL_PROFILE_VAR_NS("MyFuncs()", myfuncs); // dont start the timer
...
BL_PROFILE_VAR_START(myfuncs);
    MyFunc_0(arg);
BL_PROFILE_VAR_STOP(myfuncs);
...
BL_PROFILE_VAR_START(myfuncs);
    MyFunc_1(arg);
BL_PROFILE_VAR_STOP(myfuncs);
```

16.3 Instrumenting Fortran90 Code

When using the full profiler, Fortran90 functions can also be instrumented with the following calls:

```
call bl_proffortfuncstart("my_function")
...
call bl_proffortfuncstop("my_function")
```

Note that the start and stop calls must be matched and the profiling output will warn of any bl_proffortfuncstart calls that were not stopped with bl_proffortfuncstop calls (in debug mode only). You will need to add bl_proffortfuncstop before any returns and at the end of the function or at the point in the function you want to stop profiling.

For functions with a high number of calls, there is a lighter-weight interface:

```
call bl_proffortfuncstart_int(n)
...
call bl_proffortfuncstop_int(n)
```

where `n` is an integer in the range `[1, mFortProfsIntMaxFuncs]`. `mFortProfsIntMaxFuncs` is currently set to 32. The profiled function will be named `FORTFUNC_n` in the profiler output, unless you rename it with `BL_PROFILE_CHANGE_FORT_INT_NAME(fname, int)` where `fname` is a `std::string` and `int` is the integer `n` in the `bl_proffortfuncstart_int/bl_proffortfuncstop_int` calls. `BL_PROFILE_CHANGE_FORT_INT_NAME` should be called in `main()`.

Be aware: Fortran functions cannot be profiled when using the Tiny Profiler. You will need to turn on the full profiler to receive the results from fortran instrumentation.

16.4 Sample Output From Tiny Profile

Sample output using `TINY_PROFILE = TRUE` can look like the following:

```
TinyProfiler total time across processes [min...avg...max]: 1.765...1.765...1.765
-----
Name           NCalls   Excl. Min   Excl. Avg   Excl. Max   Max % 
-----
mfix_level::EvolveFluid      1       1.602     1.668     1.691    95.83%
FabArray::FillBoundary()    11081    0.02195    0.03336    0.06617   3.75%
FabArrayBase::getFB()        22162    0.02031    0.02147    0.02275   1.29%
PC<...>::WriteAsciiFile()   1       0.00292    0.004072   0.004551   0.26% 

-----
Name           NCalls   Incl. Min   Incl. Avg   Incl. Max   Max % 
-----
mfix_level::Evolve()         1       1.69      1.723     1.734    98.23%
mfix_level::EvolveFluid      1       1.69      1.723     1.734    98.23%
FabArray::FillBoundary()    11081    0.04236    0.05485    0.08826   5.00%
FabArrayBase::getFB()        22162    0.02031    0.02149    0.02275   1.29%
```

16.5 AMRProfParser

`AMRProfParser` is a tool for processing and analyzing the `bl_prof` database. It is a command line application that can create performance summaries, plotfiles showing point to point communication and timelines, HTML call trees, communication call statistics, function timing graphs, and other data products. The parser's data services functionality can be called from an interactive environment such as Amrvis, from a sidecar for dynamic performance optimization, and from other utilities such as the command line version of the parser itself. It has been integrated into Amrvis for visual interpretation of the data allowing Amrvis to open the `bl_prof` database like a plotfile but with interfaces appropriate to profiling data. `AMRProfParser` and `Amrvis` can be run in parallel both interactively and in batch mode.

EXTERNAL PROFILING TOOLS

17.1 CrayPat

The profiling suite available on Cray XC systems is Cray Performance Measurement and Analysis Tools (“CrayPat”)¹. Most CrayPat functionality is supported for all compilers available in the Cray “programming environments” (modules which begin “PrgEnv-”); however, a few features, chiefly the “Reveal” tool, are supported only on applications compiled with Cray’s compiler CCE²³.

CrayPat supports both high-level profiling tools, as well as fine-grained performance analysis, such as reading hardware counters. The default behavior uses sampling to identify the most time-consuming functions in an application.

17.1.1 High-level application profiling

The simplest way to obtain a high-level overview of an application’s performance consists of the following steps:

1. Load the `perftools-base` module, then the `perftools-lite` module. (The modules will not work if loaded in the opposite order.)
2. Compile the application with the Cray compiler wrappers `cc`, `CC`, and/or `ftn`. This works with any of the compilers available in the `PrgEnv-` modules. E.g., on the Cori system at NERSC, one can use the Intel, GCC, or CCE compilers. No extra compiler flags are necessary in order for CrayPat to work. CrayPat instruments the application, so the `perftools-` modules must be loaded before one compiles the application.
3. Run the application as normal. No special flags are required. Upon application completion, CrayPat will write a few files to the directory from which the application was launched. The profiling database is a single file with the `.ap2` suffix.
4. One can query the database in many different ways using the `pat_report` command on the `.ap2` file. `pat_report` is available on login nodes, so the analysis need not be done on a compute node. Querying the database with no arguments to `pat_report` prints several different profiling reports to STDOUT, including a list of the most time-consuming regions in the application. The output of this command can be long, so it can be convenient to pipe the output to a pager or a file. A portion of the output from `pat_report <file>.ap2` is shown below:

Table 1: Profile by Function

| Samp% | Samp | Imb. | Imb. | Group |
|-------|------|------|-------|----------|
| | | Samp | Samp% | Function |
| | | | | PE=HIDE |

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¹ <https://pubs.cray.com/content/S-2376/6.4.6/cray-performance-measurement-and-analysis-tools-user-guide-646-s-2376>

² <https://pubs.cray.com/content/S-2179/8.5/cray-c-and-c++-reference-manual-85>

³ <https://pubs.cray.com/content/S-3901/8.5/cray-fortran-reference-manual-85>

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| | | | | |
|--|---------|-------|-------|---------------------------------------|
| 100.0% | 5,235.5 | -- | -- | Total |
| <hr/> | | | | |
| 50.2% | 2,628.5 | -- | -- | USER |
| <hr/> | | | | |
| 7.3% | 383.0 | 15.0 | 5.0% | eos_module_mp_iterate_ne_ |
| 5.7% | 300.8 | 138.2 | 42.0% | amrex_deposit_cic |
| 5.1% | 265.2 | 79.8 | 30.8% | update_dm_particles |
| 2.8% | 147.2 | 5.8 | 5.0% | fort_fab_setval |
| 2.6% | 137.2 | 48.8 | 34.9% | amrex::ParticleContainer<>::Where |
| 2.6% | 137.0 | 11.0 | 9.9% | ppm_module_mp_ppm_type1_ |
| 2.5% | 133.0 | 24.0 | 20.4% | eos_module_mp_nyx_eos_t_given_re_ |
| 2.1% | 107.8 | 33.2 | 31.4% | amrex::ParticleContainer<> |
| <i>↳::IncrementWithTotal</i> | | | | |
| 1.7% | 89.2 | 19.8 | 24.2% | f_rhs_ |
| 1.4% | 74.0 | 7.0 | 11.5% | riemannus_ |
| 1.1% | 56.0 | 2.0 | 4.6% | amrex::VisMF::Write |
| 1.0% | 50.5 | 1.5 | 3.8% | amrex::VisMF::Header::CalculateMinMax |
| <hr/> | | | | |
| 28.1% | 1,471.0 | -- | -- | ETC |
| <hr/> | | | | |
| 7.4% | 388.8 | 10.2 | 3.4% | __intel_mic_avx512f_memcpy |
| 6.9% | 362.5 | 45.5 | 14.9% | CVode |
| 3.1% | 164.5 | 8.5 | 6.6% | __libm_log10_19 |
| 2.9% | 149.8 | 29.2 | 21.8% | _INTERNAL_25_____src_kmp_barrier_cpp_ |
| <i>↳5de9139b::__kmp_hyper_barrier_gather</i> | | | | |
| <hr/> | | | | |
| 16.8% | 879.8 | -- | -- | MPI |
| <hr/> | | | | |
| 5.1% | 266.0 | 123.0 | 42.2% | MPI_Allreduce |
| 4.2% | 218.2 | 104.8 | 43.2% | MPI_Waitall |
| 2.9% | 151.8 | 78.2 | 45.4% | MPI_Bcast |
| 2.6% | 135.0 | 98.0 | 56.1% | MPI_Barrier |
| 2.0% | 105.8 | 5.2 | 6.3% | MPI_Recv |
| <hr/> | | | | |
| 1.9% | 98.2 | -- | -- | IO |
| <hr/> | | | | |
| 1.8% | 93.8 | 6.2 | 8.3% | read |
| <hr/> | | | | |

17.2 IPM - Cross-Platform Integrated Performance Monitoring

IPM provides portable profiling capabilities across HPC platforms, including support on selected Cray and IBM machines (cori and (TODO: verify it works on) summit). Running an IPM instrumented binary generates a summary of number of calls and time spent on MPI communication library functions. In addition, hardware performance counters can also be collected through PAPI.

Detailed instructions can be found at⁴ and⁵.

⁴ <http://ipm-hpc.sourceforge.net/userguide.html>

⁵ <https://www.nersc.gov/users/software/performance-and-debugging-tools/ipm/>

17.2.1 Building with IPM on cori

Steps:

1. Run module load ipm.
2. Build code as normal with make.
3. Re-run the link command (e.g. cut-and-paste) with \$IPM added to the end of the line.

17.2.2 Running with IPM on cori

1. Set environment variables: `export IPM_REPORT=full IPM_LOG=full IPM_LOGDIR= <dir>`
2. Results will be printed to stdout and an xml file generated in the directory specified by `IPM_LOGDIR`.
3. Post-process the xml with `ipm_parse -html <xmlfile>`, which produces an directory with html.

17.2.3 Summary MPI Profile

Example MPI profile output:

```
##IPMv2.0.5#####
#
# command   : /global/cscratch1/sd/cchan2/projects/lbl/BoxLib/Tests/LinearSolvers/C_
˓→CellMG./main3d.intel.MPI.OMP.ex.ipm inputs.3d.25600
# start     : Tue Aug 15 17:34:23 2017 host       : nid11311
# stop      : Tue Aug 15 17:34:35 2017 wallclock : 11.54
# mpi_tasks : 128 on 32 nodes           %comm      : 32.51
# mem [GB]  : 126.47                 gflop/sec : 0.00
#
#          : [total]    <avg>      min      max
# wallclock : 1188.42    9.28      8.73    11.54
# MPI       : 386.31     3.02      2.51     4.78
# %wall    :
# MPI       :                   32.52     24.36    41.44
# #calls   :
# MPI       : 5031172    39306    23067    57189
# mem [GB]  : 126.47     0.99      0.98     1.00
#
#          : [time]    [count]    <%wall>
# MPI_Allreduce  225.72  567552    18.99
# MPI_Waitall   92.84  397056     7.81
# MPI_Recv      29.36   193       2.47
# MPI_Isend     25.04  2031810   2.11
# MPI_Irecv     4.35   2031810   0.37
# MPI_Allgather 2.60    128       0.22
# MPI_Barrier   2.24    512       0.19
# MPI_Gatherv   1.70    128       0.14
# MPI_Comm_dup  1.23    256       0.10
# MPI_Bcast     1.14    256       0.10
# MPI_Send      0.06    319       0.01
# MPI_Reduce   0.02    128       0.00
# MPI_Comm_free 0.01    128       0.00
# MPI_Comm_group 0.00    128       0.00
# MPI_Comm_size  0.00    256       0.00
# MPI_Comm_rank 0.00    256       0.00
```

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| | | | |
|----------------|------|-----|------|
| # MPI_Init | 0.00 | 128 | 0.00 |
| # MPI_Finalize | 0.00 | 128 | 0.00 |

The total, average, minimum, and maximum wallclock and MPI times across ranks is shown. The memory footprint is also collected. Finally, results include number of calls and total time spent in each type of MPI call.

17.2.4 PAPI Performance Counters

To collect performance counters, set `IPM_HPM=<list>`, where the list is a comma-separated list of PAPI counters. For example: `export IPM_HPM=PAPI_L2_TCA,PAPI_L2_TCM`.

For reference, here is the list of available counters on cori, which can be found by running `papi_avail`:

| Name | Code | Avail | Deriv | Description (Note) |
|--------------|------------|-------|-------|--|
| PAPI_L1_DCM | 0x80000000 | Yes | No | Level 1 data cache misses |
| PAPI_L1_ICM | 0x80000001 | Yes | No | Level 1 instruction cache misses |
| PAPI_L1_TCM | 0x80000006 | Yes | Yes | Level 1 cache misses |
| PAPI_L2_TCM | 0x80000007 | Yes | No | Level 2 cache misses |
| PAPI_TLB_DM | 0x80000014 | Yes | No | Data translation lookaside buffer misses |
| PAPI_L1_LDM | 0x80000017 | Yes | No | Level 1 load misses |
| PAPI_L2_LDM | 0x80000019 | Yes | No | Level 2 load misses |
| PAPI_STL_ICY | 0x80000025 | Yes | No | Cycles with no instruction issue |
| PAPI_BR_UCN | 0x8000002a | Yes | Yes | Unconditional branch instructions |
| PAPI_BR_CN | 0x8000002b | Yes | No | Conditional branch instructions |
| PAPI_BR_TKN | 0x8000002c | Yes | No | Conditional branch instructions taken |
| PAPI_BR_NTK | 0x8000002d | Yes | Yes | Conditional branch instructions not taken |
| PAPI_BR_MSP | 0x8000002e | Yes | No | Conditional branch instructions mispredicted |
| PAPI_TOT_INS | 0x80000032 | Yes | No | Instructions completed |
| PAPI_LD_INS | 0x80000035 | Yes | No | Load instructions |
| PAPI_SR_INS | 0x80000036 | Yes | No | Store instructions |
| PAPI_BR_INS | 0x80000037 | Yes | No | Branch instructions |
| PAPI_RES_STL | 0x80000039 | Yes | No | Cycles stalled on any resource |
| PAPI_TOT_CYC | 0x8000003b | Yes | No | Total cycles |
| PAPI_LST_INS | 0x8000003c | Yes | Yes | Load/store instructions completed |
| PAPI_L1_DCA | 0x80000040 | Yes | Yes | Level 1 data cache accesses |
| PAPI_L1_ICH | 0x80000049 | Yes | No | Level 1 instruction cache hits |
| PAPI_L1_ICA | 0x8000004c | Yes | No | Level 1 instruction cache accesses |
| PAPI_L2_TCH | 0x80000056 | Yes | Yes | Level 2 total cache hits |
| PAPI_L2_TCA | 0x80000059 | Yes | No | Level 2 total cache accesses |
| PAPI_REF_CYC | 0x8000006b | Yes | No | Reference clock cycles |

Due to hardware limitations, there is a limit to which counters can be collected simultaneously in a single run. Some counters may map to the same registers and thus cannot be collected at the same time.

17.2.5 Example HTML Performance Summary

Running `ipm_parse -html <xmlfile>` on the generated xml file will produce an HTML document that includes summary performance numbers and automatically generated figures. Some examples are shown here.

| <p>6470883</p> <ul style="list-style-type: none"> Load Balance Communication Balance Measure Buffer Sizes Measure Network Topology Switch Traffic Memory Usage Host List Environment Info Deadline Info <p>powered by IPM</p> | command: /global/cscratch1/sd/cchan2/projects/lbl/BoxLib/Tests/LinearSolvers/C_CellMG//main3d.intel.MPIOMP.ex.ipm inputs.3d.15456 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|--|--|---|---------------|---------------|-----------|-------------|-------------|-------|--------------|---------------|---------------|-------------|-----------|--------------|--------------|---------------|--------|---|-------|-----------|-----------|-------|---------------|----|------|-------|-----------|-----------|------|---------------|---|-------|-------|-----------|-----------|------|-------------|---------|-----|-------|-----------|-----------|------|-------------|---------|-----|-------|-----------|-----------|------|-------------|---------|-----|-------|-----------|-----------|------|-------------|--------|-----|-------|-----------|-----------|------|-------------|---------|-----|-------|-----------|-----------|------|-------------|-------|------|-------|-----------|-----------|------|-------------|-------|-----|-------|-----------|-----------|------|-------------|--------|-----|-------|-----------|-----------|------|-------------|--------|-----|-------|-----------|-----------|------|-------------|--------|-----|-------|-----------|-----------|------|-------------|-------|-----|-------|-----------|-----------|------|-----------|-----|---|-------|-----------|-----------|------|-------------|--------|-----|-------|-----------|-----------|------|-----------|-------|------|-------|-----------|-----------|------|-------------|---|----|-------|-----------|-----------|------|
| | codename: | unknown state: | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | username: | cchan2 group: | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | host: | nid04720 (x86_64 Linux) mpi_tasks: 4 on 1 hosts | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | start: | 08/22/17/12:04:29 wallclock: 5.20833e+01 sec | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | stop: | 08/22/17/12:05:20 %comm: 4.99170175468912 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | total memory: | 28.82264 gbytes total gflop/sec: 0 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | switch(send): | 0 gbytes switch(recv): 0 gbytes | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | Computation | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | Communication | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | <table border="1"> <thead> <tr> <th>Event</th> <th>Count</th> <th>Pop</th> </tr> </thead> <tbody> <tr> <td>PAPI L2_TCA</td> <td>1884011012</td> <td>*</td> </tr> <tr> <td>PAPI L2_TCM</td> <td>447288209</td> <td>*</td> </tr> </tbody> </table> | | Event | Count | Pop | PAPI L2_TCA | 1884011012 | * | PAPI L2_TCM | 447288209 | * | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Event | Count | Pop | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PAPI L2_TCA | 1884011012 | * | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PAPI L2_TCM | 447288209 | * | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| HPM Counter Statistics <table border="1"> <thead> <tr> <th>Event</th> <th>Ntasks</th> <th>Avg</th> <th>Min(rank)</th> <th>Max(rank)</th> </tr> </thead> <tbody> <tr> <td>PAPI L2_TCA</td> <td>*</td> <td>471002753.00</td> <td>418954739 (2)</td> <td>558450816 (3)</td> </tr> <tr> <td>PAPI L2_TCM</td> <td>*</td> <td>111822052.25</td> <td>83963410 (2)</td> <td>172440952 (3)</td> </tr> </tbody> </table> | | Event | Ntasks | Avg | Min(rank) | Max(rank) | PAPI L2_TCA | * | 471002753.00 | 418954739 (2) | 558450816 (3) | PAPI L2_TCM | * | 111822052.25 | 83963410 (2) | 172440952 (3) | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Event | Ntasks | Avg | Min(rank) | Max(rank) | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PAPI L2_TCA | * | 471002753.00 | 418954739 (2) | 558450816 (3) | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| PAPI L2_TCM | * | 111822052.25 | 83963410 (2) | 172440952 (3) | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Communication Event Statistics (100.00% detail, 6.9785e-06 error) <table border="1"> <thead> <tr> <th>Buffer Size</th> <th>Nealls</th> <th>Total Time</th> <th>Min Time</th> <th>Max Time</th> <th>%MPI</th> <th>%Wall</th> </tr> </thead> <tbody> <tr><td>MPI_Waitall</td><td>0</td><td>5360</td><td>5.774</td><td>1.788e-05</td><td>2.530e-02</td><td>55.53</td></tr> <tr><td>MPI_Gatherv</td><td>114688</td><td>4</td><td>1.257</td><td>4.390e-01</td><td>4.390e-01</td><td>12.09</td></tr> <tr><td>MPI_Allreduce</td><td>16</td><td>1908</td><td>0.684</td><td>1.288e-05</td><td>1.238e-02</td><td>6.58</td></tr> <tr><td>MPI_Allreduce</td><td>8</td><td>10900</td><td>0.611</td><td>6.914e-06</td><td>3.187e-03</td><td>5.88</td></tr> <tr><td>MPI_Waitall</td><td>4194304</td><td>302</td><td>0.435</td><td>1.044e-03</td><td>9.893e-03</td><td>4.18</td></tr> <tr><td>MPI_Waitall</td><td>3670016</td><td>151</td><td>0.338</td><td>8.841e-04</td><td>1.869e-01</td><td>3.25</td></tr> <tr><td>MPI_Waitall</td><td>2621440</td><td>151</td><td>0.176</td><td>8.039e-04</td><td>2.057e-02</td><td>1.69</td></tr> <tr><td>MPI_Waitall</td><td>917504</td><td>135</td><td>0.160</td><td>3.550e-04</td><td>4.294e-02</td><td>1.54</td></tr> <tr><td>MPI_Waitall</td><td>1048576</td><td>270</td><td>0.157</td><td>2.749e-04</td><td>3.719e-03</td><td>1.51</td></tr> <tr><td>MPI_Waitall</td><td>65536</td><td>1838</td><td>0.112</td><td>5.198e-05</td><td>4.921e-04</td><td>1.07</td></tr> <tr><td>MPI_Waitall</td><td>57344</td><td>919</td><td>0.095</td><td>5.293e-05</td><td>1.865e-02</td><td>0.92</td></tr> <tr><td>MPI_Waitall</td><td>655360</td><td>135</td><td>0.082</td><td>2.880e-04</td><td>1.567e-02</td><td>0.79</td></tr> <tr><td>MPI_Waitall</td><td>229376</td><td>135</td><td>0.066</td><td>1.240e-04</td><td>2.626e-02</td><td>0.64</td></tr> <tr><td>MPI_Waitall</td><td>262144</td><td>270</td><td>0.063</td><td>1.280e-04</td><td>1.812e-03</td><td>0.61</td></tr> <tr><td>MPI_Waitall</td><td>40960</td><td>919</td><td>0.062</td><td>4.482e-05</td><td>1.561e-02</td><td>0.60</td></tr> <tr><td>MPI_Bcast</td><td>320</td><td>4</td><td>0.049</td><td>1.639e-02</td><td>1.639e-02</td><td>0.47</td></tr> <tr><td>MPI_Waitall</td><td>163840</td><td>135</td><td>0.043</td><td>9.584e-05</td><td>1.981e-02</td><td>0.41</td></tr> <tr><td>MPI_Isend</td><td>20480</td><td>3676</td><td>0.032</td><td>1.907e-06</td><td>9.990e-05</td><td>0.31</td></tr> <tr><td>MPI_Barrier</td><td>0</td><td>16</td><td>0.027</td><td>4.540e-04</td><td>5.476e-03</td><td>0.26</td></tr> </tbody> </table> | | Buffer Size | Nealls | Total Time | Min Time | Max Time | %MPI | %Wall | MPI_Waitall | 0 | 5360 | 5.774 | 1.788e-05 | 2.530e-02 | 55.53 | MPI_Gatherv | 114688 | 4 | 1.257 | 4.390e-01 | 4.390e-01 | 12.09 | MPI_Allreduce | 16 | 1908 | 0.684 | 1.288e-05 | 1.238e-02 | 6.58 | MPI_Allreduce | 8 | 10900 | 0.611 | 6.914e-06 | 3.187e-03 | 5.88 | MPI_Waitall | 4194304 | 302 | 0.435 | 1.044e-03 | 9.893e-03 | 4.18 | MPI_Waitall | 3670016 | 151 | 0.338 | 8.841e-04 | 1.869e-01 | 3.25 | MPI_Waitall | 2621440 | 151 | 0.176 | 8.039e-04 | 2.057e-02 | 1.69 | MPI_Waitall | 917504 | 135 | 0.160 | 3.550e-04 | 4.294e-02 | 1.54 | MPI_Waitall | 1048576 | 270 | 0.157 | 2.749e-04 | 3.719e-03 | 1.51 | MPI_Waitall | 65536 | 1838 | 0.112 | 5.198e-05 | 4.921e-04 | 1.07 | MPI_Waitall | 57344 | 919 | 0.095 | 5.293e-05 | 1.865e-02 | 0.92 | MPI_Waitall | 655360 | 135 | 0.082 | 2.880e-04 | 1.567e-02 | 0.79 | MPI_Waitall | 229376 | 135 | 0.066 | 1.240e-04 | 2.626e-02 | 0.64 | MPI_Waitall | 262144 | 270 | 0.063 | 1.280e-04 | 1.812e-03 | 0.61 | MPI_Waitall | 40960 | 919 | 0.062 | 4.482e-05 | 1.561e-02 | 0.60 | MPI_Bcast | 320 | 4 | 0.049 | 1.639e-02 | 1.639e-02 | 0.47 | MPI_Waitall | 163840 | 135 | 0.043 | 9.584e-05 | 1.981e-02 | 0.41 | MPI_Isend | 20480 | 3676 | 0.032 | 1.907e-06 | 9.990e-05 | 0.31 | MPI_Barrier | 0 | 16 | 0.027 | 4.540e-04 | 5.476e-03 | 0.26 |
| Buffer Size | Nealls | Total Time | Min Time | Max Time | %MPI | %Wall | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 0 | 5360 | 5.774 | 1.788e-05 | 2.530e-02 | 55.53 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Gatherv | 114688 | 4 | 1.257 | 4.390e-01 | 4.390e-01 | 12.09 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Allreduce | 16 | 1908 | 0.684 | 1.288e-05 | 1.238e-02 | 6.58 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Allreduce | 8 | 10900 | 0.611 | 6.914e-06 | 3.187e-03 | 5.88 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 4194304 | 302 | 0.435 | 1.044e-03 | 9.893e-03 | 4.18 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 3670016 | 151 | 0.338 | 8.841e-04 | 1.869e-01 | 3.25 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 2621440 | 151 | 0.176 | 8.039e-04 | 2.057e-02 | 1.69 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 917504 | 135 | 0.160 | 3.550e-04 | 4.294e-02 | 1.54 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 1048576 | 270 | 0.157 | 2.749e-04 | 3.719e-03 | 1.51 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 65536 | 1838 | 0.112 | 5.198e-05 | 4.921e-04 | 1.07 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 57344 | 919 | 0.095 | 5.293e-05 | 1.865e-02 | 0.92 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 655360 | 135 | 0.082 | 2.880e-04 | 1.567e-02 | 0.79 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 229376 | 135 | 0.066 | 1.240e-04 | 2.626e-02 | 0.64 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 262144 | 270 | 0.063 | 1.280e-04 | 1.812e-03 | 0.61 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 40960 | 919 | 0.062 | 4.482e-05 | 1.561e-02 | 0.60 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Bcast | 320 | 4 | 0.049 | 1.639e-02 | 1.639e-02 | 0.47 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Waitall | 163840 | 135 | 0.043 | 9.584e-05 | 1.981e-02 | 0.41 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Isend | 20480 | 3676 | 0.032 | 1.907e-06 | 9.990e-05 | 0.31 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MPI_Barrier | 0 | 16 | 0.027 | 4.540e-04 | 5.476e-03 | 0.26 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

Fig. 17.1: Sample performance summary generated by IPM

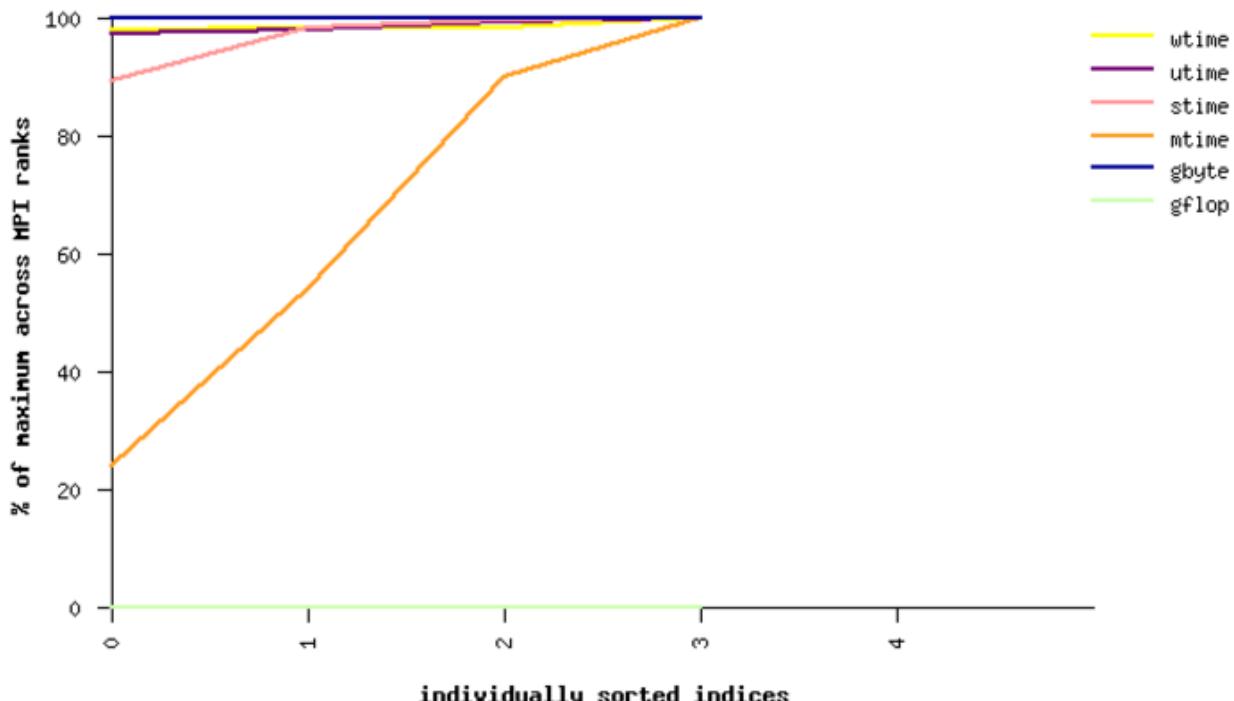
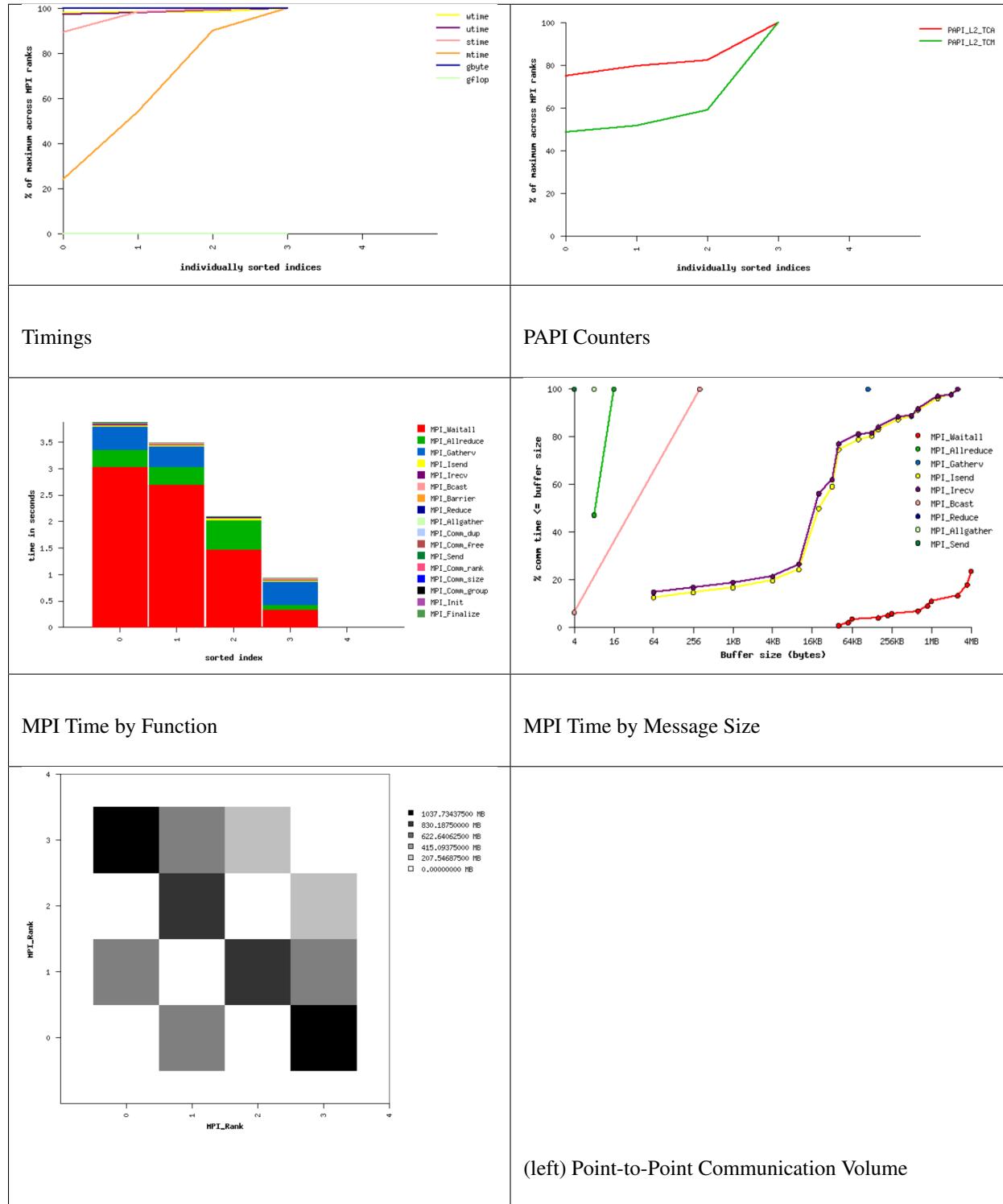


Table 17.1: Example of performance graphs generated by IPM



CHAPTER
EIGHTEEN

EXTERNAL FRAMEWORKS

18.1 CVODE

AMReX supports local ODE integration using the CVODE solver,¹ which is part of the SUNDIALS framework.² CVODE contains solvers for stiff and non-stiff ODEs, and as such is well suited for solving e.g., the complex chemistry networks in combustion simulations, or the nuclear reaction networks in astrophysical simulations.

Most of CVODE is written in C, but many functions also come with two distinct Fortran interfaces. One interface is FCVODE, which is bundled with the stable release of CVODE. Its usage is described in the CVODE documentation.³ However, the use of FCVODE is discouraged in AMReX due to its incompatibility with being used inside OpenMP parallel regions (which is the primary use case in AMReX applications).

The alternative, and recommended, Fortran interface to uses the `iso_c_binding` feature of the Fortran 2003 standard to implement a direct interface to the C functions in CVODE. When compiling CVODE, one need not build the CVODE library with the FCVODE interface enabled at all. Rather, the Fortran 2003 interface to CVODE is provided within AMReX itself. The CVODE tutorials provided in AMReX use this new interface.

18.1.1 Compiling AMReX with CVODE (Cray or Sundials version 2.7)

The following steps describe how to compile an AMReX application with CVODE support. On Cray systems (e.g., Cori or Edison at NERSC), Cray provides a system module called `cray-tpsl` (“Cray Third-Party Scientific Libraries”) which contains the latest version of the SUNDIALS solver suite (including CVODE). Simply type `module load cray-tpsl` and set `USE_CVODE=TRUE` in the `GNUmakefile`, and AMReX will automatically link the SUNDIALS libraries.

On systems which are not Cray:

1. Obtain the CVODE source code, which is hosted here: <https://computation.llnl.gov/projects/sundials/sundials-software>. One can download either the complete SUNDIALS package, or just the CVODE components.
2. Unpack the CVODE / SUNDIALS tarball, and create a new “build” directory (it can be anywhere).
3. Navigate to the new, empty build directory, and type

```
cmake \
-DCMAKE_INSTALL_PREFIX:PATH=/path/to/install/dir \
/path/to/cvode/or/sundials/top/level/source/dir
```

¹ <https://computation.llnl.gov/projects/sundials/cvode>

² <https://computation.llnl.gov/projects/sundials>

³ https://computation.llnl.gov/sites/default/files/public/cv_guide.pdf

The CMAKE_INSTALL_DIR option tells CMake where to install the libraries. Note that CMake will attempt to deduce the compilers automatically, but respects certain environment variables if they are defined, such as CC (for the C compiler), CXX (for the C++ compiler), and FC (for the Fortran compiler). So one may modify the above CMake invocation to be something like the following:

```
CC=/path/to/gcc \
CXX=/path/to/g++ \
FC=/path/to/gfortran \
cmake \
-DCMAKE_INSTALL_PREFIX:PATH=/path/to/install/dir \
/path/to/cvode/or/sundials/top/level/source/dir
```

One can supply additional flags to CMake or to the compiler to customize the compilation process. Flags of interest may include CMAKE_C_FLAGS, which add the specified flags to the compile statement, e.g., `-DCMAKE_C_FLAGS="-h list=a"` will append the `-h list=a` flag to the `cc` statement when compiling the source code. Here one may wish to add something like `"-O2 -g"` to provide an optimized library that still contains debugging symbols; if one neglects debugging symbols in the CVODE library, and if a code that uses CVODE encounters a segmentation fault in the solve, then the backtrace has no information about where in the solver the error occurred. Also, if one wishes to compile only the solver library itself and not the examples that come with the source (compiling the examples is enabled by default), one can add `"-DEXAMPLES_ENABLE=OFF"`. Users should be aware that the CVODE examples are linked dynamically, so when compiling the solver library on Cray system using the Cray compiler wrappers `cc`, `CC`, and `ftn`, one should explicitly disable compiling the examples via the `"-DEXAMPLES_ENABLE=OFF"` flag.

4. In the GNUmakefile for the application which uses the Fortran 2003 interface to , add `USE_CVODE = TRUE`, which will compile the Fortran 2003 interfaces and link the libraries. Note that one must define the `CVODE_LIB_DIR` environment variable to point to the location where the libraries are installed.

18.1.2 CVODE Tutorials

AMReX provides two CVODE tutorials in the `amrex/Tutorials/CVODE` directory, called EX1 and EX2. See the Tutorials `CVODE` documentation for more detail.

18.1.3 Compiling AMReX with Sundials version 3.X or later

The following steps describe how to compile an AMReX application with SUNDIALS_3.X support. On Cray systems (e.g., Cori or Edison at NERSC), Cray provides a system module called `cray-tpsl` (“Cray Third-Party Scientific Libraries”) which as of this writing contains the 2.7 version of the SUNDIALS solver suite (including CVODE).

In order to use the Sundials 3.X version:

1. Obtain the CVODE source code, which is hosted here: <https://computation.llnl.gov/projects/sundials/sundials-software>. One can download either the complete SUNDIALS package, or just the CVODE components.
2. Unpack the CVODE / SUNDIALS tarball, and create a new “build” directory (it can be anywhere).
3. Navigate to the new, empty build directory, and type

```
cmake \
-DCMAKE_INSTALL_PREFIX:PATH=/path/to/install/dir \
/path/to/cvode/or/sundials/top/level/source/dir
```

The CMAKE_INSTALL_DIR option tells CMake where to install the libraries. Note that CMake will attempt to deduce the compilers automatically, but respects certain environment variables if they are defined, such as CC

(for the C compiler), CXX (for the C++ compiler), and FC (for the Fortran compiler). So one may modify the above CMake invocation to be something like the following:

```
CC=/path/to/gcc \
CXX=/path/to/g++ \
FC=/path/to/gfortran \
cmake \
-DCMAKE_INSTALL_PREFIX:PATH=/path/to/install/dir \
/path/to/cvode/or/sundials/top/level/source/dir
```

One can supply additional flags to CMake or to the compiler to customize the compilation process. Flags of interest may include CMAKE_C_FLAGS, which add the specified flags to the compile statement, e.g., -DCMAKE_C_FLAGS="-h list=a" will append the -h list=a flag to the cc statement when compiling the source code. Here one may wish to add something like "-O2 -g" to provide an optimized library that still contains debugging symbols; if one neglects debugging symbols in the CVODE library, and if a code that uses CVODE encounters a segmentation fault in the solve, then the backtrace has no information about where in the solver the error occurred. Also, if one wishes to compile only the solver library itself and not the examples that come with the source (compiling the examples is enabled by default), one can add "-DEXAMPLES_ENABLE=OFF". Users should be aware that the CVODE examples are linked dynamically, so when compiling the solver library on Cray system using the Cray compiler wrappers cc, CC, and ftn, one should explicitly disable compiling the examples via the "-DEXAMPLES_ENABLE=OFF" flag.

4. In the `GNUmakefile` for the application which uses the Fortran 2003 interface to CVODE or ARKODE, add `SUNDIALS_3x4x = TRUE`, which will compile the Fortran 2003 interfaces and link the libraries. Note that one must define the `CVODE_LIB_DIR` environment variable to point to the location where the libraries are installed.
5. In the `GNUmakefile` for the application which uses the Fortran 2003 interface to ARKODE, also add `USE_ARKODE_LIBS = TRUE`. It is assumed that the `CVODE_LIB_DIR` environment variable points to the location where the ARKODE libraries are installed as well.
6. Fortran 2003 interfaces for the pgi compilers and for developmental versions of SUNDIALS are currently not supported.

18.1.4 SUNDIALS 3.X Tutorials

AMReX provides six tutorials in the `amrex/Tutorials/CVODE/SUNDIALS3_finterface` directory. EX1 is modeled after the CVODE Tutorial EX1 showing use with AMReX. The four `EX_cv_*` tutorials are based on examples provided with the interface, which are more closely modeled after CVODE examples. The `EX_ark_analytic_fp` tutorial is based on the `EX_cv_analytic_fp` tutorial, but uses ARKODE instead of CVODE.

AMReX provides three tutorials in the `amrex/Tutorials/CVODE/SUNDIALS3_cppversion` directory. These are versions of EX1 which operate on a packed version of the data. `EX1_SERIAL_NVEC` packs a box worth of equations into a serial NVector, uses CVODE to solve, and then unpacks the solution back into the box it came from. `EX1_CUDA_NVEC` uses the cuda NVector implementation instead. `EX1_GPU_PRAGMA` uses the cuda NVector, and the gpu pragma functionality.

18.2 SWFFT

`hacc/SWFFT`, developed by Adrian Pope et al. at Argonne National Lab, provides the functionality to perform forward and reverse Fast Fourier Transforms (FFT) within a fully parallelized framework built in C++ and F90. In the

words of HACC’s developers, SWFFT is a “distributed-memory, pencil-decomposed, parallel 3D FFT.”¹ The SWFFT source code is also contained in the following directory within AMReX: amrex/Src/Extern/SWFFT.²

18.2.1 Pencil Redistribution

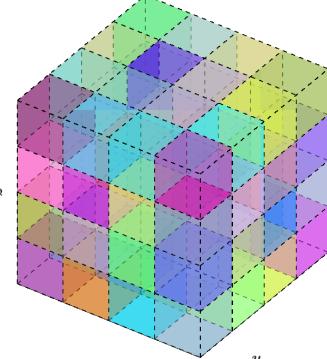
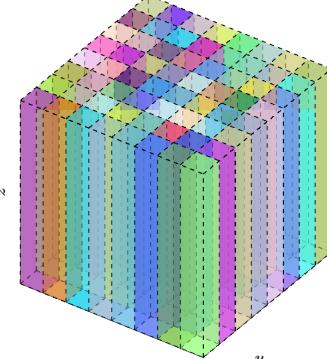
As input, SWFFT takes three-dimensional arrays of data distributed across block-structured grids, and redistributes the data into “pencil” grids in z , x , and then y , belonging to different MPI processes. After each pencil conversion, a 1D FFT is performed on the data along the pencil direction using calls to the FFTW³ library. The README files in the tutorial directories specify the relationship between the number of grids and the number of MPI processes that should be used. The hacc/SWFFT README document by Adrian Pope et al. explains restrictions on grid dimensions in relation to the number of MPI processes¹²:

[...] A rule of thumb is that [SWFFT] generally works when the number of vertexes along one side of the global 3D grid (“ng”) can be factored into small primes, and when the number of MPI ranks can also be factored into small primes. I believe that all of the unique prime factors of the number of MPI ranks must be present in the set of prime factors of the grid, eg. if you have 20 MPI ranks then ng must be a multiple of 5 and 2. The CheckDecomposition utility is provided to check (on one rank) whether a proposed grid size and number of MPI ranks will work, which can be done before submitting a large test with TestDfft/TestFDfft.

The relationship between the number of processes versus global grid dimensions is determined by how the total number of grids can be factored from a three dimensional grid structure (block structured grids) into a two dimensional structure (pencil arrays), as shown in the figures below.

The following figures illustrate how data is distributed from block structured grids to pencil arrays within SWFFT, where the colors of each box indicate which MPI rank it belongs to:

Table 18.1: SWFFT Redistribution from $4 \times 4 \times 4$ Box Array into Pencils

| | |
|--|--|
|  (a) Block structured grids: $N_x = 4, N_y = 4, N_z = 4$ |  (b) Z-pencils: $N_x = 8, N_y = 8, N_z = 1$ |
|--|--|

¹ <https://xgitlab.cels.anl.gov/hacc/SWFFT>

² SWFFT source code directory in AMReX: amrex/Src/Extern/SWFFT

³ <http://www.fftw.org/>

Table 18.2: SWFFT Redistribution from $2 \times 2 \times 2$ Box Array into Pencils

| | | |
|---|--|--|
| | | |
| (a) Block structured grids: $N_x = 2, N_y = 2, N_z = 2$ | | (b) Z-pencils: $N_x = 4, N_y = 2, N_z = 1$ |
| | | |
| (c) X-pencils: $N_x = 1, N_y = 4, N_z = 2$ | | (d) Y-pencils: $N_x = 4, N_y = 1, N_z = 2$ |

Using the same number of AMReX grids as processes has been verified to work in the `SWFFT_poisson` and `SWFFT_simple` tutorials. This can be illustrated by the following equation for the total number of grids, N_b , in a regularly structured domain:

$$N_b = m_{bi}m_{bj} = n_{bi}n_{bj}n_{bk},$$

where n_{bi} , n_{bj} , and n_{bk} are the number of grids, or boxes, in the x , y , and z dimensions of the block-structured grid. Analogously, for pencil distributions, m_{bi} and m_{bj} are the number of grids along the remaining dimensions if pencils are taken in the k direction. There are many possible ways of redistributing the data, for example $m_{bi} = n_{bi}n_{bk}$ & $m_{bj} = n_{bj}$ is one possible simple configuration. However, it is evident from the figures above that the SWFFT redistribution algorithm has a more sophisticated method for finding the prime factors of the grid.

18.2.2 Tutorials

AMReX contains two SWFFT tutorials, `SWFFT_poisson` and `SWFFT_simple`:

- `SWFFT_poisson` tutorial: The tutorial found in `amrex/Tutorials/SWFFT/SWFFT_poisson` solves a Poisson equation with periodic boundary conditions. In it, both a forward FFT and reverse FFT are called to solve the equation, however, no reordering of the DFT data in k-space is performed.
- `SWFFT_simple` tutorial: This tutorial: `amrex/Tutorials/SWFFT/SWFFT_simple`, is useful if the objective is to simply take a forward FFT of data, and the DFT's ordering in k-space matters to the user. This tutorial initializes a 3D or 2D `MultiFab`, takes a forward FFT, and then redistributes the data in k-space back to the “correct,” 0 to 2π , ordering. The results are written to a plot file.

CHAPTER
NINETEEN

INDICES AND TABLES

- genindex
- modindex
- search

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