Earth System Modeling Framework

ESMF Reference Manual for C

Version 8.7.0 beta snapshot

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http://www.earthsystemmodeling.org

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Contents

Part I

ESMF Overview

1 What is the Earth System Modeling Framework?

The Earth System Modeling Framework (ESMF) is a suite of software tools for developing high-performance, multi-component Earth science modeling applications. Such applications may include a few or dozens of components representing atmospheric, oceanic, terrestrial, or other physical domains, and their constituent processes (dynamical, chemical, biological, etc.). Often these components are developed by different groups independently, and must be "coupled" together using software that transfers and transforms data among the components in order to form functional simulations.

ESMF supports the development of these complex applications in a number of ways. It introduces a set of simple, consistent component interfaces that apply to all types of components, including couplers themselves. These interfaces expose in an obvious way the inputs and outputs of each component. It offers a variety of data structures for transferring data between components, and libraries for regridding, time advancement, and other common modeling functions. Finally, it provides a growing set of tools for using metadata to describe components and their input and output fields. This capability is important because components that are self-describing can be integrated more easily into automated workflows, model and dataset distribution and analysis portals, and other emerging "semantically enabled" computational environments.

ESMF is not a single Earth system model into which all components must fit, and its distribution doesn't contain any scientific code. Rather it provides a way of structuring components so that they can be used in many different user-written applications and contexts with minimal code modification, and so they can be coupled together in new configurations with relative ease. The idea is to create many components across a broad community, and so to encourage new collaborations and combinations.

ESMF offers the flexibility needed by this diverse user base. It is tested nightly on more than two dozen platform/compiler combinations; can be run on one processor or thousands; supports shared and distributed memory programming models and a hybrid model; can run components sequentially (on all the same processors) or concurrently (on mutually exclusive processors); and supports single executable or multiple executable modes.

ESMF's generality and breadth of function can make it daunting for the novice user. To help users navigate the software, we try to apply consistent names and behavior throughout and to provide many examples. The large-scale structure of the software is straightforward. The utilities and data structures for building modeling components are called the ESMF *infrastructure*. The coupling interfaces and drivers are called the *superstructure*. User code sits between these two layers, making calls to the infrastructure libraries underneath and being scheduled and synchronized by the superstructure above. The configuration resembles a sandwich, as shown in Figure 1.

ESMF users may choose to extensively rewrite their codes to take advantage of the ESMF infrastructure, or they may decide to simply wrap their components in the ESMF superstructure in order to utilize framework coupling services. Either way, we encourage users to contact our support team if questions arise about how to best use the software, or how to structure their application. ESMF is more than software; it's a group of people dedicated to realizing the vision of a collaborative model development community that spans institutional and national bounds.

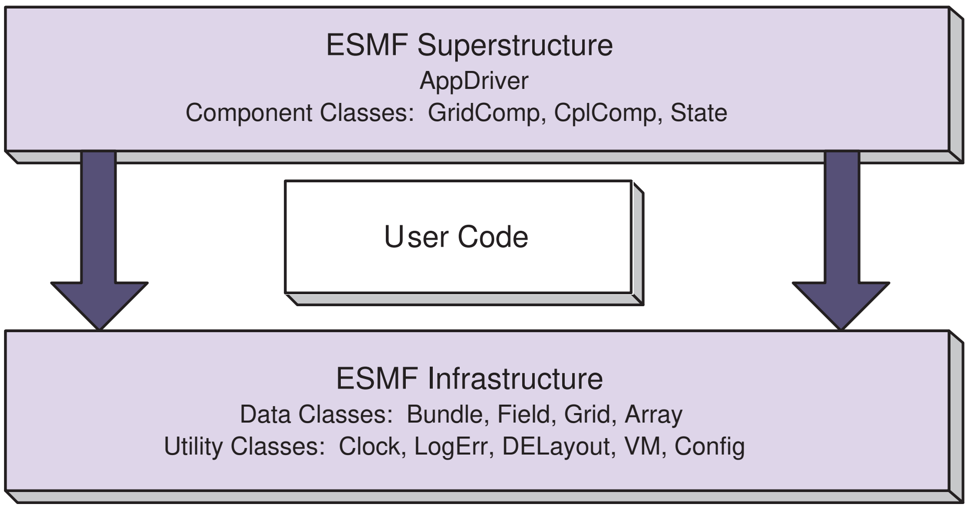
2 The ESMF Reference Manual for C

ESMF has a complete set of Fortran interfaces and some C interfaces. This *ESMF Reference Manual* is a listing of ESMF interfaces for C.

Interfaces are grouped by class. A class is comprised of the data and methods for a specific concept like a physical field. Superstructure classes are listed first in this *Manual*, followed by infrastructure classes.

The major classes in the ESMF superstructure are Components, which usually represent large pieces of functionality such as atmosphere and ocean models, and States, which are the data structures used to transfer data between

Figure 1: Schematic of the ESMF "sandwich" architecture. The framework consists of two parts, an upper level **superstructure** layer and a lower level **infrastructure** layer. User code is sandwiched between these two layers.



Components. There are both data structures and utilities in the ESMF infrastructure. Data structures include multi-dimensional Arrays, Fields that are comprised of an Array and a Grid, and collections of Arrays and Fields called ArrayBundles and FieldBundles, respectively. There are utility libraries for data decomposition and communications, time management, logging and error handling, and application configuration.

3 How to Contact User Support and Find Additional Information

The ESMF team can answer questions about the interfaces presented in this document. For user support, please contact esmf_support@ucar.edu.

The website, http://www.earthsystemmodeling.org, provide more information of the ESMF project as a whole. The website includes release notes and known bugs for each version of the framework, supported platforms, project history, values, and metrics, related projects, the ESMF management structure, and more. The *ESMF User's Guide* contains build and installation instructions, an overview of the ESMF system and a description of how its classes interrelate (this version of the document corresponds to the last public version of the framework). Also available on the ESMF website is the *ESMF Developer's Guide* that details ESMF procedures and conventions.

4 How to Submit Comments, Bug Reports, and Feature Requests

We welcome input on any aspect of the ESMF project. Send questions and comments to esmf_support@ucar.edu.

5 The ESMF Application Programming Interface

The ESMF Application Programming Interface (API) is based on the object-oriented programming concept of a **class**. A class is a software construct that is used for grouping a set of related variables together with the subroutines and functions that operate on them. We use classes in ESMF because they help to organize the code, and often make it easier to maintain and understand. A particular instance of a class is called an **object**. For example, Field is an ESMF class. An actual Field called temperature is an object. That is about as far as we will go into software engineering terminology.

The C interface is implemented so that the variables associated with a class are stored in a C structure. For example, an ESMC_Field structure stores the data array, grid information, and metadata associated with a physical field. The structure for each class is defined in a C header file. The operations associated with each class are also defined in the header files.

The header files for ESMF are bundled together and can be accessed with a single include statement, #include "ESMC.h". By convention, the C entry points are named using "ESMC" as a prefix.

5.1 Standard Methods and Interface Rules

ESMF defines a set of standard methods and interface rules that hold across the entire API. These are:

- ESMC_<Class>Create() and ESMC_<Class>Destroy(), for creating and destroying objects of ESMF classes that require internal memory management (- called ESMF deep classes). The ESMC_<Class>Create() method allocates memory for the object itself and for internal variables, and initializes variables where appropriate. It is always written as a function that returns a derived type instance of the class, i.e. an object.
- ESMC_<Class>Set() and ESMC_<Class>Get(), for setting and retrieving a particular item or flag. In general, these methods are overloaded for all cases where the item can be manipulated as a name/value pair. If identifying the item requires more than a name, or if the class is of sufficient complexity that overloading in this way would result in an overwhelming number of options, we define specific ESMC_<Class>Set<Something>() and ESMC_<Class>Get<Something>() interfaces.
- ESMC_<Class>Add(), ESMC_<Class>AddReplace(), ESMC_<Class>Remove(), and ESMC_<Class>Replace(), for manipulating objects of ESMF container classes - such as ESMC_State and ESMC_FieldBundle. For example, the ESMC_FieldBundleAdd() method adds another Field to an existing FieldBundle object.
- ESMC_<Class>Print(), for printing the contents of an object to standard out. This method is mainly intended for debugging.
- ESMC_<Class>ReadRestart() and ESMC_<Class>WriteRestart(), for saving the contents of a class and restoring it exactly. Read and write restart methods have not yet been implemented for most ESMF classes, so where necessary the user needs to write restart values themselves.
- ESMC_<Class>Validate(), for determining whether a class is internally consistent. For example, ESMC_FieldValidate() validates the internal consistency of a Field object.

5.2 Deep and Shallow Classes

ESMF contains two types of classes.

Deep classes require `ESMC_<Class>Create()` and `ESMC_<Class>Destroy()` calls. They involve memory allocation, take significant time to set up (due to memory management) and should not be created in a time-critical portion of code. Deep objects persist even after the method in which they were created has returned. Most classes in ESMF, including GridComp, CplComp, State, Fields, FieldBundles, Arrays, ArrayBundles, Grids, and Clocks, fall into this category.

Shallow classes do not possess `ESMC_<Class>Create()` and `ESMC_<Class>Destroy()` calls. They are simply declared and their values set using an `ESMC_<Class>Set()` call. Examples of shallow classes are Time, TimeInterval, and ArraySpec. Shallow classes do not take long to set up and can be declared and set within a time-critical code segment. Shallow objects stop existing when execution goes out of the declaring scope.

An exception to this is when a shallow object, such as a Time, is stored in a deep object such as a Clock. The deep Clock object then becomes the declaring scope of the Time object, persisting in memory. The Time object is deallocated with the `ESMC_ClockDestroy()` call.

See Section 8, Overall Design and Implementation Notes, for a brief discussion of deep and shallow classes from an implementation perspective. For an in-depth look at the design and inter-language issues related to deep and shallow classes, see the *ESMF Implementation Report*.

5.3 Aliases

Deep objects, i.e. instances of ESMF deep classes created by the appropriate `ESMC_<Class>Create()`, can be used with the standard assignment (=) operator.

The assignment

```
deep2 = deep1
```

makes `deep2` an **alias** of `deep1`, meaning that both variables reference the same deep allocation in memory. Many aliases of the same deep object can be created.

All the aliases of a deep object are equivalent. In particular, there is no distinction between the variable on the left hand side of the actual `ESMC_<Class>Create()` call, and any aliases created from it. All actions taken on any of the aliases of a deep object affect the deep object, and thus all other aliases.

5.4 Special Methods

The following are special methods which, in one case, are required by any application using ESMF, and in the other case must be called by any application that is using ESMF Components.

- `ESMC_Initialize()` and `ESMC_Finalize()` are required methods that must bracket the use of ESMF within an application. They manage the resources required to run ESMF and shut it down gracefully. ESMF does not support restarts in the same executable, i.e. `ESMC_Initialize()` should not be called after `ESMC_Finalize()`.
- `ESMC_<Type>CompInitialize()`, `ESMC_<Type>CompRun()`, and `ESMC_<Type>CompFinalize()` are component methods that are used at the highest level within ESMF. `<Type>` may be `<Grid>`, for Gridded Components such as oceans or atmospheres, or `<Cpl>`, for Coupler Components that are used to connect them. The content of these methods is not part of the ESMF. Instead the methods call into associated subroutines within user code.

5.5 The ESMF Data Hierarchy

The ESMF API is organized around a hierarchy of classes that contain model data. The operations that are performed on model data, such as regridding, redistribution, and halo updates, are methods of these classes.

The main data classes offered by the ESMF C API, in order of increasing complexity, are:

- **Array** An ESMF Array is a distributed, multi-dimensional array that can carry information such as its type, kind, rank, and associated halo widths. It contains a reference to a native language array.
- **Field** A Field represents a physical scalar or vector field. It contains a reference to an Array along with grid information and metadata.
- **State** A State represents the collection of data that a Component either requires to run (an Import State) or can make available to other Components (an Export State). States may contain references to Arrays, ArrayBundles, Fields, FieldBundles, or other States.
- **Component** A Component is a piece of software with a distinct function. ESMF currently recognizes two types of Components. Components that represent a physical domain or process, such as an atmospheric model, are called Gridded Components since they are usually discretized on an underlying grid. The Components responsible for regridding and transferring data between Gridded Components are called Coupler Components. Each Component is associated with an Import and an Export State. Components can be nested so that simpler Components are contained within more complex ones.

Underlying these data classes are native language arrays. ESMF Arrays and Fields can be queried for the C pointer to the actual data. You can perform communication operations either on the ESMF data objects or directly on C arrays through the VM class, which serves as a unifying wrapper for distributed and shared memory communication libraries.

5.6 ESMF Spatial Classes

Like the hierarchy of model data classes, ranging from the simple to the complex, ESMF is organized around a hierarchy of classes that represent different spaces associated with a computation. Each of these spaces can be manipulated, in order to give the user control over how a computation is executed. For Earth system models, this hierarchy starts with the address space associated with the computer and extends to the physical region described by the application. The main spatial classes in ESMF, from those closest to the machine to those closest to the application, are:

- The **Virtual Machine**, or **VM** The ESMF VM is an abstraction of a parallel computing environment that encompasses both shared and distributed memory, single and multi-core systems. Its primary purpose is resource allocation and management. Each Component runs in its own VM, using the resources it defines. The elements of a VM are **Persistent Execution Threads**, or **PETs**, that are executing in **Virtual Address Spaces**, or **VASs**. A simple case is one in which every PET is associated with a single MPI process. In this case every PET is executing in its own private VAS. If Components are nested, the parent Component allocates a subset of its PETs to its children. The children have some flexibility, subject to the constraints of the computing environment, to decide how they want to use the resources associated with the PETs they've received.
- **DELayout** A DELayout represents a data decomposition (we also refer to this as a distribution). Its basic elements are **Decomposition Elements**, or **DEs**. A DELayout associates a set of DEs with the PETs in a VM. DEs are not necessarily one-to-one with PETs. For cache blocking, or user-managed multi-threading, more DEs than PETs may be defined. Fewer DEs than PETs may also be defined if an application requires it.

  The current ESMF C API does not provide user access to the DELayout class.

- **DistGrid** A DistGrid represents the index space associated with a grid. It is a useful abstraction because often a full specification of grid coordinates is not necessary to define data communication patterns. The DistGrid contains information about the sequence and connectivity of data points, which is sufficient information for many operations. Arrays are defined on DistGrids.
- **Array** An Array defines how the index space described in the DistGrid is associated with the VAS of each PET. This association considers the type, kind and rank of the indexed data. Fields are defined on Arrays.
- **Grid** A Grid is an abstraction for a logically rectangular region in physical space. It associates a coordinate system, a set of coordinates, and a topology to a collection of grid cells. Grids in ESMF are comprised of DistGrids plus additional coordinate information.
- **Mesh** A Mesh provides an abstraction for an unstructured grid. Coordinate information is set in nodes, which represent vertices or corners. Together the nodes establish the boundaries of mesh elements or cells.
- **LocStream** A LocStream is an abstraction for a set of unstructured data points without any topological relationship to each other.
- **Field** A Field may contain more dimensions than the Grid that it is discretized on. For example, for convenience during integration, a user may want to define a single Field object that holds snapshots of data at multiple times. Fields also keep track of the stagger location of a Field data point within its associated Grid cell.

5.7 ESMF Maps

In order to define how the index spaces of the spatial classes relate to each other, we require either implicit rules (in which case the relationship between spaces is defined by default), or special Map arrays that allow the user to specify the desired association. The form of the specification is usually that the position of the array element carries information about the first object, and the value of the array element carries information about the second object. ESMF includes a `distGridToArrayMap`, a `gridToFieldMap`, a `distGridToGridMap`, and others.

5.8 ESMF Specification Classes

It can be useful to make small packets of descriptive parameters. ESMF has one of these:

- **ArraySpec**, for storing the specifics, such as type/kind/rank, of an array.

5.9 ESMF Utility Classes

There are a number of utilities in ESMF that can be used independently. These are:

- **Attributes**, for storing metadata about Fields, FieldBundles, States, and other classes. (Not currently available through the ESMF C API.)
- **TimeMgr**, for calendar, time, clock and alarm functions.
- **LogErr**, for logging and error handling.
- **Config**, for creating resource files that can replace namelists as a consistent way of setting configuration parameters.

6 Integrating ESMF into Applications

Depending on the requirements of the application, the user may want to begin integrating ESMF in either a top-down or bottom-up manner. In the top-down approach, tools at the superstructure level are used to help reorganize and structure the interactions among large-scale components in the application. It is appropriate when interoperability is a primary concern; for example, when several different versions or implementations of components are going to be swapped in, or a particular component is going to be used in multiple contexts. Another reason for deciding on a top-down approach is that the application contains legacy code that for some reason (e.g., intertwined functions, very large, highly performance-tuned, resource limitations) there is little motivation to fully restructure. The superstructure can usually be incorporated into such applications in a way that is non-intrusive.

In the bottom-up approach, the user selects desired utilities (data communications, calendar management, performance profiling, logging and error handling, etc.) from the ESMF infrastructure and either writes new code using them, introduces them into existing code, or replaces the functionality in existing code with them. This makes sense when maximizing code reuse and minimizing maintenance costs is a goal. There may be a specific need for functionality or the component writer may be starting from scratch. The calendar management utility is a popular place to start.

6.1 Using the ESMF Superstructure

The following is a typical set of steps involved in adopting the ESMF superstructure. The first two tasks, which occur before an ESMF call is ever made, have the potential to be the most difficult and time-consuming. They are the work of splitting an application into components and ensuring that each component has well-defined stages of execution. ESMF aside, this sort of code structure helps to promote application clarity and maintainability, and the effort put into it is likely to be a good investment.

1. Decide how to organize the application as discrete Gridded and Coupler Components. This might involve reorganizing code so that individual components are cleanly separated and their interactions consist of a minimal number of data exchanges.
2. Divide the code for each component into initialize, run, and finalize methods. These methods can be multi-phase, e.g., `init_1, init_2`.
3. Pack any data that will be transferred between components into ESMF Import and Export State data structures. This is done by first wrapping model data in either ESMF Arrays or Fields. Arrays are simpler to create and use than Fields, but carry less information and have a more limited range of operations. These Arrays and Fields are then added to Import and Export States. They may be packed into ArrayBundles or FieldBundles first, for more efficient communications. Metadata describing the model data can also be added. At the end of this step, the data to be transferred between components will be in a compact and largely self-describing form.
4. Pack time information into ESMF time management data structures.
5. Using code templates provided in the ESMF distribution, create ESMF Gridded and Coupler Components to represent each component in the user code.
6. Write a set services routine that sets ESMF entry points for each user component's initialize, run, and finalize methods.
7. Run the application using an ESMF Application Driver.

6.2 Constants

Named constants are used throughout ESMF to specify the values of many arguments with multiple well defined values in a consistent way. These constants are defined by a derived type that follows this pattern:

```
ESMF_<CONSTANT_NAME>_Flag
```

The values of the constant are then specified by this pattern:

```
ESMF_<CONSTANT_NAME>_<VALUE1>
ESMF_<CONSTANT_NAME>_<VALUE2>
ESMF_<CONSTANT_NAME>_<VALUE3>
...
```

A master list of all available constants can be found in section **??**.

7 Overall Rules and Behavior

7.1 Local and Global Views and Associated Conventions

ESMF data objects such as Fields are distributed over DEs, with each DE getting a portion of the data. Depending on the task, a local or global view of the object may be preferable. In a local view, data indices start with the first element on the DE and end with the last element on the same DE. In a global view, there is an assumed or specified order to the set of DEs over which the object is distributed. Data indices start with the first element on the first DE, and continue across all the elements in the sequence of DEs. The last data index represents the number of elements in the entire object. The DistGrid provides the mapping between local and global data indices.

The convention in ESMF is that entities with a global view have no prefix. Entities with a DE-local (and in some cases, PET-local) view have the prefix "local."

Just as data is distributed over DEs, DEs themselves can be distributed over PETs. This is an advanced feature for users who would like to create multiple local chunks of data, for algorithmic or performance reasons. Local DEs are those DEs that are located on the local PET. Local DE labeling always starts at 0 and goes to localDeCount-1, where localDeCount is the number of DEs on the local PET. Global DE numbers also start at 0 and go to deCount-1. The DELayout class provides the mapping between local and global DE numbers.

7.2 Allocation Rules

The basic rule of allocation and deallocation for the ESMF is: whoever allocates it is responsible for deallocating it.

ESMF methods that allocate their own space for data will deallocate that space when the object is destroyed. Methods which accept a user-allocated buffer, for example `ESMC_FieldCreate()` with the `ESMF_DATACOPY_REFERENCE` flag, will not deallocate that buffer at the time the object is destroyed. The user must deallocate the buffer when all use of it is complete.

Classes such as Fields, FieldBundles, and States may have Arrays, Fields, Grids and FieldBundles created externally and associated with them. These associated items are not destroyed along with the rest of the data object since it is possible for the items to be added to more than one data object at a time (e.g. the same Grid could be part of many Fields). It is the user's responsibility to delete these items when the last use of them is done.

7.3 Assignment, Equality, Copying and Comparing Objects

The equal sign assignment has not been overloaded in ESMF, thus resulting in the standard C behavior. This behavior has been documented as the first entry in the API documentation section for each ESMF class. For deep ESMF objects the assignment results in setting an alias the the same ESMF object in memory. For shallow ESMF objects the assignment is essentially a equivalent to a copy of the object. For deep classes the equality operators have been overloaded to test for the alias condition as a counter part to the assignment behavior. This and the not equal operator are documented following the assignment in the class API documentation sections.

Deep object copies are implemented as a special variant of the ESMC_<Class>Create() methods. It takes an existing deep object as one of the required arguments. At this point not all deep classes have ESMC_<Class>Create() methods that allow object copy.

Due to the complexity of deep classes there are many aspects when comparing two objects of the same class. ESMF provide ESMC_<Class>Match() methods, which are functions that return a class specific match flag. At this point not all deep classes have ESMC_<Class>Match() methods that allow deep object comparison.

8 Overall Design and Implementation Notes

1. **Deep and shallow classes.** The deep and shallow classes described in Section 5.2 differ in how and where they are allocated within a multi-language implementation environment. We distinguish between the implementation language, which is the language a method is written in, and the calling language, which is the language that the user application is written in. Deep classes are allocated off the process heap by the implementation language. Shallow classes are allocated off the stack by the calling language.

2. **Base class.** All ESMF classes are built upon a Base class, which holds a small set of system-wide capabilities.

Part II

Command Line Tools

The main product delivered by ESMF is the ESMF library that allows application developers to write programs based on the ESMF API. In addition to the programming library, ESMF distributions come with a small set of command line tools (CLT) that are of general interest to the community. These CLTs utilize the ESMF library to implement features such as printing general information about the ESMF installation, or generating regrid weight files. The provided ESMF CLTs are intended to be used as standard command line tools.

The bundled ESMF CLTs are built and installed during the usual ESMF installation process, which is described in detail in the ESMF User's Guide section "Building and Installing the ESMF". After installation, the CLTs will be located in the `ESMF_APPSDIR` directory, which can be found as a Makefile variable in the `esmf.mk` file. The `esmf.mk` file can be found in the `ESMF_INSTALL_LIBDIR` directory after a successful installation. The ESMF User's Guide discusses the `esmf.mk` mechanism to access the bundled CLTs in more detail in section "Using Bundled ESMF Command Line Tools".

The following sections provide in-depth documentation of the bundled ESMF CLTs. In addition, each tool supports the standard `--help` command line argument, providing a brief description of how to invoke the program.

Part III

Superstructure

9 Overview of Superstructure

ESMF superstructure classes define an architecture for assembling Earth system applications from modeling **components**. A component may be defined in terms of the physical domain that it represents, such as an atmosphere or sea ice model. It may also be defined in terms of a computational function, such as a data assimilation system. Earth system research often requires that such components be **coupled** together to create an application. By coupling we mean the data transformations and, on parallel computing systems, data transfers, that are necessary to allow data from one component to be utilized by another. ESMF offers regridding methods and other tools to simplify the organization and execution of inter-component data exchanges.

In addition to components defined at the level of major physical domains and computational functions, components may be defined that represent smaller computational functions within larger components, such as the transformation of data between the physics and dynamics in a spectral atmosphere model, or the creation of nested higher resolution regions within a coarser grid. The objective is to couple components at varying scales both flexibly and efficiently. ESMF encourages a hierarchical application structure, in which large components branch into smaller sub-components (see Figure 2). ESMF also makes it easier for the same component to be used in multiple contexts without changes to its source code.

Key Features
Modular, component-based architecture.
Hierarchical assembly of components into applications.
Use of components in multiple contexts without modification.
Sequential or concurrent component execution.
Single program, multiple datastream (SPMD) applications for maximum portability and reconfigurability.
Multiple program, multiple datastream (MPMD) option for flexibility.

9.1 Superstructure Classes

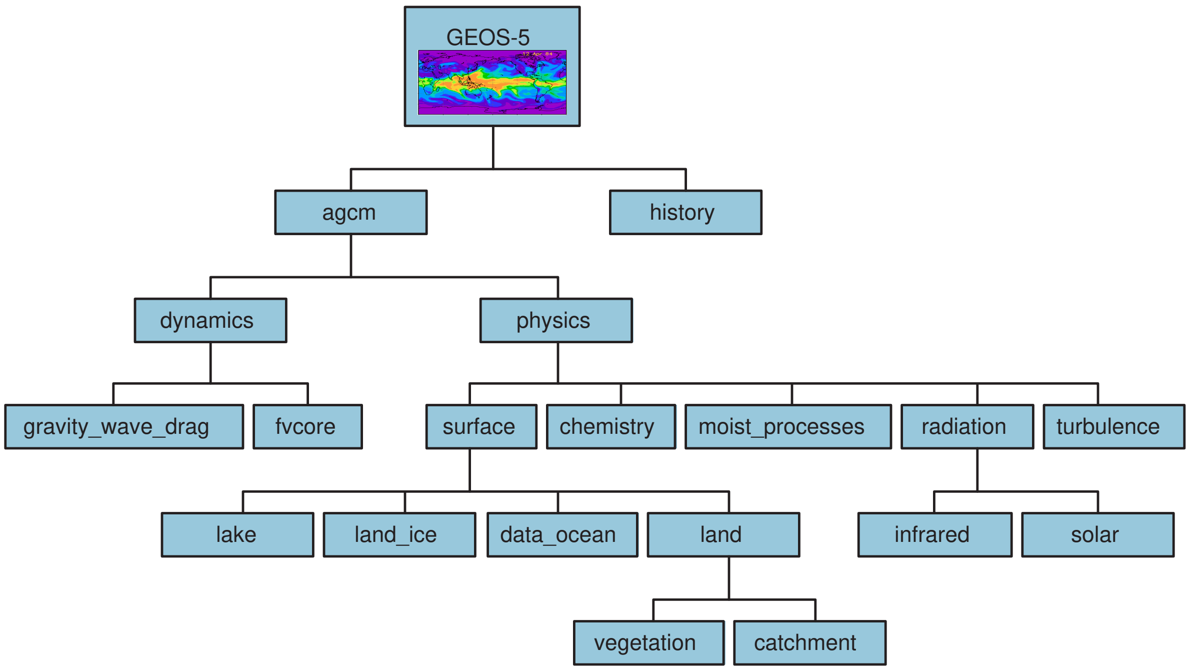
There are a small number of classes in the ESMF superstructure:

- **Component** An ESMF component has two parts, one that is supplied by ESMF and one that is supplied by the user. The part that is supplied by the framework is an ESMF derived type that is either a Gridded Component (**GridComp**) or a Coupler Component (**CplComp**). A Gridded Component typically represents a physical domain in which data is associated with one or more grids - for example, a sea ice model. A Coupler Component arranges and executes data transformations and transfers between one or more Gridded Components. Gridded Components and Coupler Components have standard methods, which include initialize, run, and finalize. These methods can be multi-phase.

  The second part of an ESMF Component is user code, such as a model or data assimilation system. Users set entry points within their code so that it is callable by the framework. In practice, setting entry points means that within user code there are calls to ESMF methods that associate the name of a Fortran subroutine with a corresponding standard ESMF operation. For example, a user-written initialization routine called `myOceanInit` might be associated with the standard initialize routine of an ESMF Gridded Component named “myOcean” that represents an ocean model.

- **State** ESMF Components exchange information with other Components only through States. A State is an ESMF derived type that can contain Fields, FieldBundles, Arrays, ArrayBundles, and other States. A Component is associated with two States, an **Import State** and an **Export State**. Its Import State holds the data that it receives from other Components. Its Export State contains data that it makes available to other Components.

Figure 2: ESMF enables applications such as the atmospheric general circulation model GEOS-5 to be structured hierarchically, and reconfigured and extended easily. Each box in this diagram is an ESMF Gridded Component.



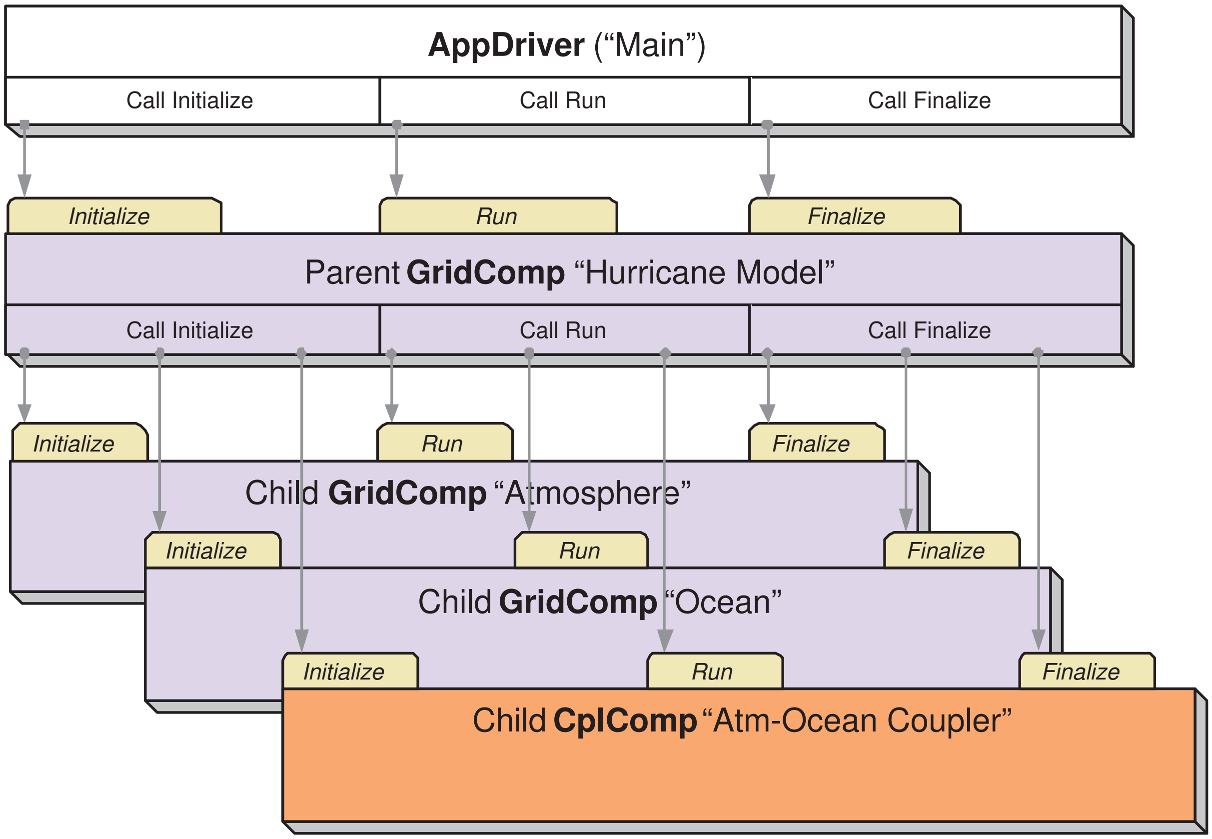
An ESMF coupled application typically involves a parent Gridded Component, two or more child Gridded Components and one or more Coupler Components.

The parent Gridded Component is responsible for creating the child Gridded Components that are exchanging data, for creating the Coupler, for creating the necessary Import and Export States, and for setting up the desired sequencing. The application's "main" routine calls the parent Gridded Component's initialize, run, and finalize methods in order to execute the application. For each of these standard methods, the parent Gridded Component in turn calls the corresponding methods in the child Gridded Components and the Coupler Component. For example, consider a simple coupled ocean/atmosphere simulation. When the initialize method of the parent Gridded Component is called by the application, it in turn calls the initialize methods of its child atmosphere and ocean Gridded Components, and the initialize method of an ocean-to-atmosphere Coupler Component. Figure 3 shows this schematically.

9.2 Hierarchical Creation of Components

Components are allocated computational resources in the form of **Persistent Execution Threads**, or **PET**s. A list of a Component's PETs is contained in a structure called a **Virtual Machine**, or **VM**. The VM also contains information about the topology and characteristics of the underlying computer. Components are created hierarchically, with parent Components creating child Components and allocating some or all of their PETs to each one. By default ESMF creates a new VM for each child Component, which allows Components to tailor their VM resources to match their needs. In some cases, a child may want to share its parent's VM - ESMF supports this, too.

Figure 3: A call to a standard ESMF initialize (run, finalize) method by a parent component triggers calls to initialize (run, finalize) all of its child components.



A Gridded Component may exist across all the PETs in an application. A Gridded Component may also reside on a subset of PETs in an application. These PETs may wholly coincide with, be wholly contained within, or wholly contain another Component.

9.3 Sequential and Concurrent Execution of Components

When a set of Gridded Components and a Coupler runs in sequence on the same set of PETs the application is executing in a **sequential** mode. When Gridded Components are created and run on mutually exclusive sets of PETs, and are coupled by a Coupler Component that extends over the union of these sets, the mode of execution is **concurrent**.

Figure 4 illustrates a typical configuration for a simple coupled sequential application, and Figure 5 shows a possible configuration for the same application running in a concurrent mode.

Parent Components can select if and when to wait for concurrently executing child Components, synchronizing only when required.

It is possible for ESMF applications to contain some Component sets that are executing sequentially and others that are executing concurrently. We might have, for example, atmosphere and land Components created on the same subset of PETs, ocean and sea ice Components created on the remainder of PETs, and a Coupler created across all the PETs in the application.

9.4 Intra-Component Communication

All data transfers within an ESMF application occur *within* a component. For example, a Gridded Component may contain halo updates. Another example is that a Coupler Component may redistribute data between two Gridded Components. As a result, the architecture of ESMF does not depend on any particular data communication mechanism, and new communication schemes can be introduced without affecting the overall structure of the application.

Since all data communication happens within a component, a Coupler Component must be created on the union of the PETs of all the Gridded Components that it couples.

9.5 Data Distribution and Scoping in Components

The scope of distributed objects is the VM of the currently executing Component. For this reason, all PETs in the current VM must make the same distributed object creation calls. When a Coupler Component running on a superset of a Gridded Component's PETs needs to make communication calls involving objects created by the Gridded Component, an ESMF-supplied function called `ESMF_StateReconcile()` creates proxy objects for those PETs that had no previous information about the distributed objects. Proxy objects contain no local data but can be used in communication calls (such as regrid or redistribute) to describe the remote source for data being moved to the current PET, or to describe the remote destination for data being moved from the local PET. Figure 6 is a simple schematic that shows the sequence of events in a reconcile call.

9.6 Performance

The ESMF design enables the user to configure ESMF applications so that data is transferred directly from one component to another, without requiring that it be copied or sent to a different data buffer as an interim step. This is likely to be the most efficient way of performing inter-component coupling. However, if desired, an application can also be configured so that data from a source component is sent to a distinct set of Coupler Component PETs for processing before being sent to its destination.

The ability to overlap computation with communication is essential for performance. When running with ESMF the user can initiate data sends during Gridded Component execution, as soon as the data is ready. Computations can then proceed simultaneously with the data transfer.

Figure 4: Schematic of the run method of a coupled application, with an “Atmosphere” and an “Ocean” Gridded Component running sequentially with an “Atm-Ocean Coupler.” The top-level “Hurricane Model” Gridded Component contains the sequencing information and time advancement loop. The application driver, Coupler, and all Gridded Components are distributed over nine PETs.

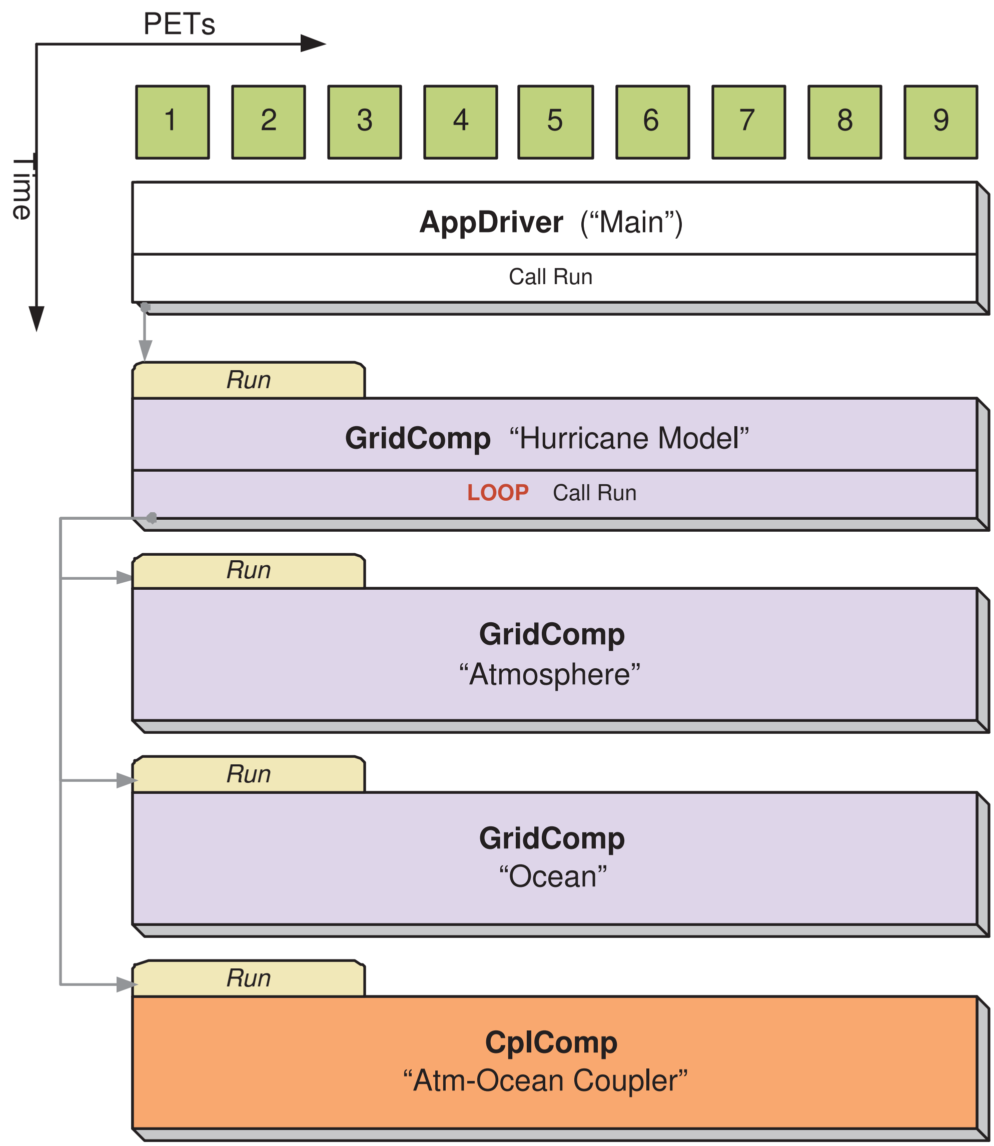


Figure 5: Schematic of the run method of a coupled application, with an "Atmosphere" and an "Ocean" Gridded Component running concurrently with an "Atm-Ocean Coupler." The top-level "Hurricane Model" Gridded Component contains the sequencing information and time advancement loop. The application driver, Coupler, and top-level "Hurricane Model" Gridded Component are distributed over nine PETs. The "Atmosphere" Gridded Component is distributed over three PETs and the "Ocean" Gridded Component is distributed over six PETs.

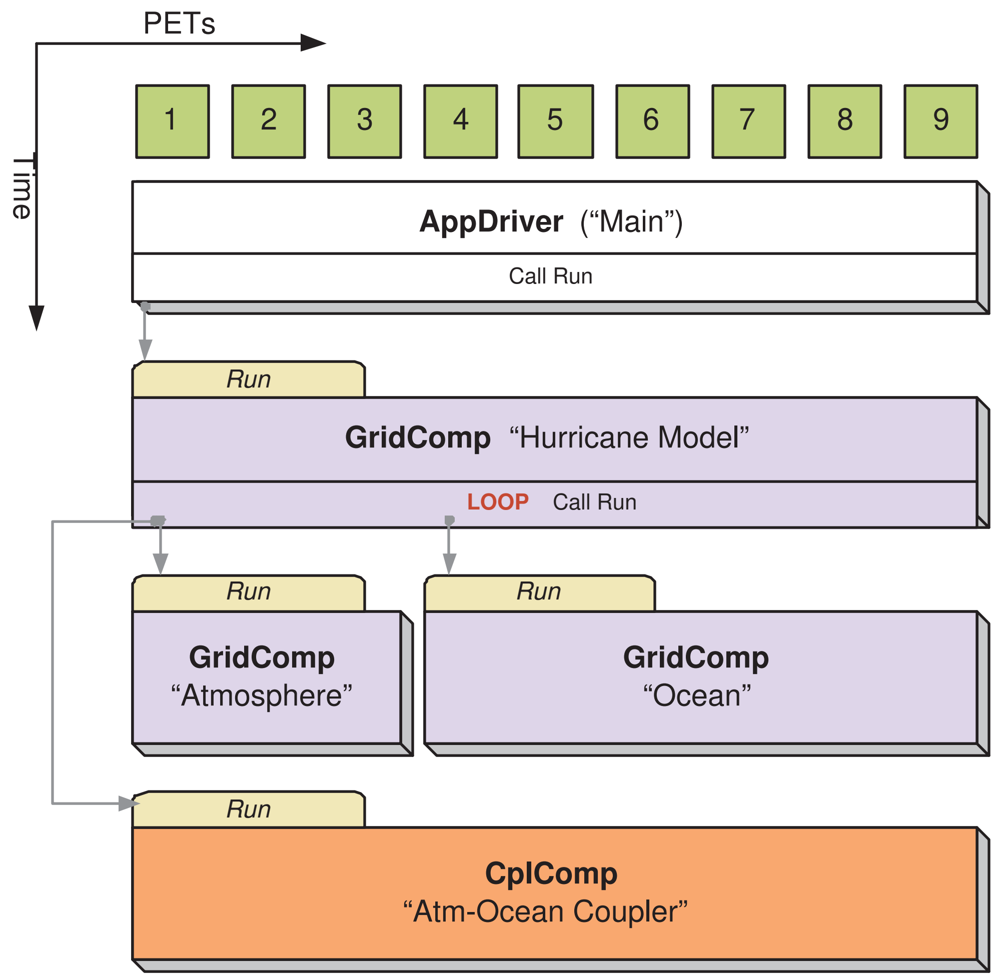
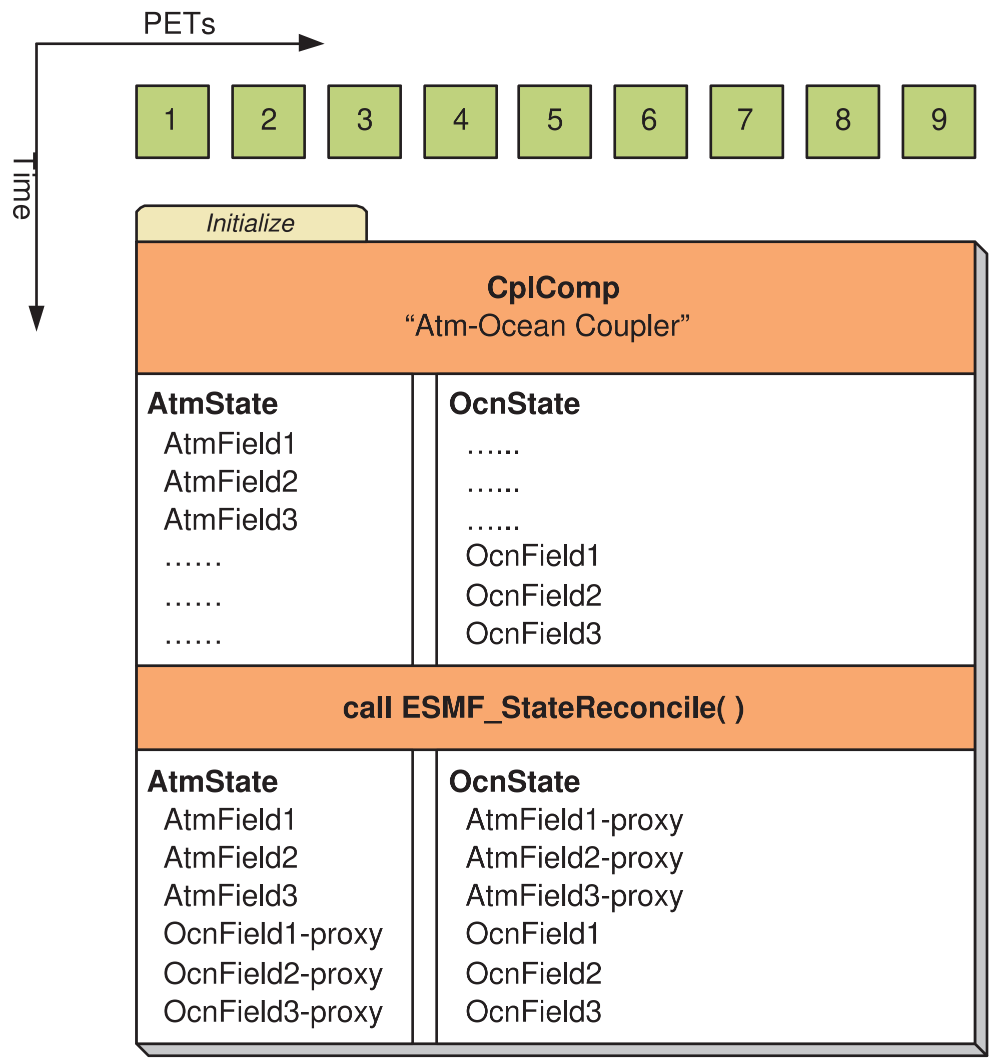
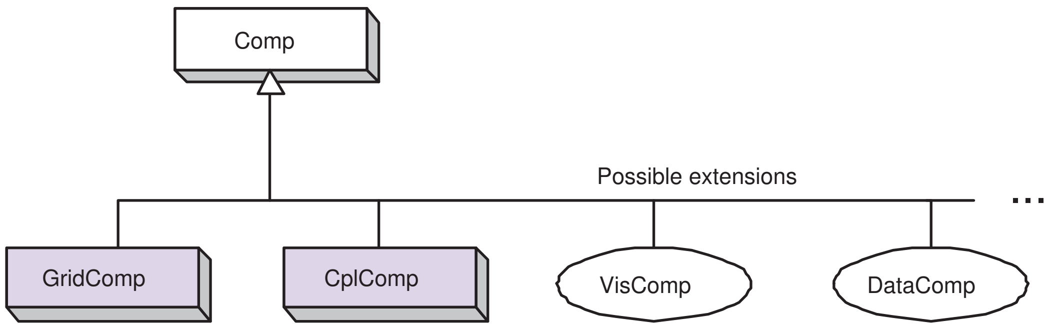


Figure 6: An `ESMF_StateReconcile()` call creates proxy objects for use in subsequent communication calls. The reconcile call would normally be made during Coupler initialization.



9.7 Object Model

The following is a simplified Unified Modeling Language (UML) diagram showing the relationships among ESMF superstructure classes. See Appendix A, *A Brief Introduction to UML*, for a translation table that lists the symbols in the diagram and their meaning.



10 Application Driver and Required ESMF Methods

10.1 Description

Every ESMF application needs a driver code. Typically the driver layer is implemented as the "main" of the application, although this is not strictly an ESMF requirement. For most ESMF applications the task of the application driver will be very generic: Initialize ESMF, create a top-level Component and call its Initialize, Run and Finalize methods, before destroying the top-level Component again and calling ESMF Finalize.

ESMF provides a number of different application driver templates in the `$ESMF_DIR/src/Superstructure/AppDriver` directory. An appropriate one can be chosen depending on how the application is to be structured:

Sequential vs. Concurrent Execution In a sequential execution model, every Component executes on all PETs, with each Component completing execution before the next Component begins. This has the appeal of simplicity of data consumption and production: when a Gridded Component starts, all required data is available for use, and when a Gridded Component finishes, all data produced is ready for consumption by the next Gridded Component. This approach also has the possibility of less data movement if the grid and data decomposition is done such that each processor's memory contains the data needed by the next Component.

In a concurrent execution model, subgroups of PETs run Gridded Components and multiple Gridded Components are active at the same time. Data exchange must be coordinated between Gridded Components so that data deadlock does not occur. This strategy has the advantage of allowing coupling to other Gridded Components at any time during the computational process, including not having to return to the calling level of code before making data available.

Pairwise vs. Hub and Spoke Coupler Components are responsible for taking data from one Gridded Component and putting it into the form expected by another Gridded Component. This might include regridding, change of units, averaging, or binning.

Coupler Components can be written for *pairwise* data exchange: the Coupler Component takes data from a single Component and transforms it for use by another single Gridded Component. This simplifies the structure of the Coupler Component code.

Couplers can also be written using a *hub and spoke* model where a single Coupler accepts data from all other Components, can do data merging or splitting, and formats data for all other Components.

Multiple Couplers, using either of the above two models or some mixture of these approaches, are also possible.

Implementation Language The ESMF framework currently has Fortran interfaces for all public functions. Some functions also have C interfaces, and the number of these is expected to increase over time.

Number of Executables The simplest way to run an application is to run the same executable program on all PETs. Different Components can still be run on mutually exclusive PETs by using branching (e.g., if this is PET 1, 2, or 3, run Component A, if it is PET 4, 5, or 6 run Component B). This is a **SPMD** model, Single Program Multiple Data.

The alternative is to start a different executable program on different PETs. This is a **MPMD** model, Multiple Program Multiple Data. There are complications with many job control systems on multiprocessor machines in getting the different executables started, and getting inter-process communications established. ESMF currently has some support for MPMD: different Components can run as separate executables, but the Coupler that transfers data between the Components must still run on the union of their PETs. This means that the Coupler Component must be linked into all of the executables.

10.2 Required ESMF Methods

There are a few methods that every ESMF application must contain. First, `ESMC_Initialize()` and `ESMC_Finalize()` are in complete analogy to `MPI_Init()` and `MPI_Finalize()` known from MPI. All ESMF programs, serial or parallel, must initialize the ESMF system at the beginning, and finalize it at the end of execution. The behavior of calling any ESMF method before `ESMC_Initialize()`, or after `ESMC_Finalize()` is undefined.

Second, every ESMF Component that is accessed by an ESMF application requires that its set services routine is called through `ESMC_<Grid/Cpl>CompSetServices()`. The Component must implement one public entry point, its set services routine, that can be called through the `ESMC_<Grid/Cpl>CompSetServices()` library routine. The Component set services routine is responsible for setting entry points for the standard ESMF Component methods Initialize, Run, and Finalize.

Finally, the Component can optionally call `ESMC_<Grid/Cpl>CompSetVM()` *before* calling `ESMC_<Grid/Cpl>CompSetServices()`. Similar to `ESMC_<Grid/Cpl>CompSetServices()`, the `ESMC_<Grid/Cpl>CompSetVM()` call requires a public entry point into the Component. It allows the Component to adjust certain aspects of its execution environment, i.e. its own VM, before it is started up.

The following sections discuss the above mentioned aspects in more detail.

10.2.1 ESMC_Initialize - Initialize ESMF

INTERFACE:

```
int ESMC_Initialize(
  int *rc,         // return code
```

```
...);            // optional arguments (see below)
```

RETURN VALUE:

```
Return code; equals ESMF_SUCCESS if there are no errors.
```

DESCRIPTION:

Initialize the ESMF. This method must be called before any other ESMF methods are used. The method contains a barrier before returning, ensuring that all processes made it successfully through initialization.

Typically `ESMC_Initialize()` will call `MPI_Init()` internally unless MPI has been initialized by the user code before initializing the framework. If the MPI initialization is left to `ESMC_Initialize()` it inherits all of the MPI implementation dependent limitations of what may or may not be done before `MPI_Init()`. For instance, it is unsafe for some MPI implementations, such as MPICH1, to do I/O before the MPI environment is initialized. Please consult the documentation of your MPI implementation for details.

Optional arguments are recognised. To indicate the end of the optional argument list, `ESMC_ArgLast` must be used. A minimal call to `ESMC_Initialize()` would be:

```
ESMC_Initialize (NULL, ESMC_ArgLast);
```

The optional arguments are specified using the `ESMC_InitArg` macros. For example, to turn off logging so that no log files would be created, the `ESMC_Initialize()` call would be coded as:

```
ESMC_Initialize (&rc,
  ESMC_InitArgLogKindFlag(ESMC_LOGKIND_NONE),
  ESMC_ArgLast);
```

Before exiting the application the user must call `ESMC_Finalize()` to release resources and clean up the ESMF gracefully.

The arguments are:

[rc] Return code; equals `ESMF_SUCCESS` if there are no errors. `NULL` may be passed when the return code is not desired.

[ESMC_InitArgDefaultCalKind(ARG)] Macro specifying the default calendar kind for the entire application. Valid values for `ARG` are documented in section **??**. If not specified, defaults to `ESMC_CALKIND_NOCALENDAR`.

[ESMC_InitArgDefaultConfigFilename(ARG)] Macro specifying the name of the default configuration file for the Config class. If not specified, no default file is used.

[ESMC_InitArgLogFilename(ARG)] Macro specifying the name used as part of the default log file name for the default log. If not specified, defaults to `ESMF_LogFile`.

[ESMC_InitArgLogKindFlag(ARG)] Macro specifying the default Log kind to be used by ESMF Log Manager. Valid values for `ARG` are documented in section **??**. If not specified, defaults to `ESMC_LOGKIND_MULTI`.

ESMC_ArgLast Macro indicating the end of the optional argument list. This must be provided even when there are no optional arguments.
