A Component-Based Approach to Integrated Modeling in the Geosciences: The Design of CSDMS

Scott Peckham, Eric Hutton

CSDMS, University of Colorado, 1560 30th Street, UCB 450, Boulder, CO 80309, USA

Boyana Norris

Mathematics and Computer Science Division, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL 60439, USA

Abstract

The development of scientific modeling software increasingly requires the coupling of multiple independently developed models. Component-based software engineering enables the integration of plug-and-play components, but significant additional challenges must be addressed in any specific domain in order to produce a usable development and simulation environment that is also going to encourage contributions and adoption by entire communities. In this paper we describe the challenges in creating a coupling environment for Earth-surface process modeling and how we approach them in our integration efforts at the Community Surface Dynamics Modeling System.

Keywords:

component software, CCA, CSDMS, modeling, code generation

Email addresses: Scott.Peckham@colorado.edu (Scott Peckham), Eric.Hutton@colorado.edu (Eric Hutton), norris@mcs.anl.gov (Boyana Norris)

1. Introduction

The Community Surface Dynamics Modeling System (CSDMS) project (CSDMS, 2011) is an NSF-funded, international effort to develop a suite of modular numerical models able to simulate a wide variety of Earth-surface processes, on time scales ranging from individual events to many millions of years. CSDMS maintains a large, searchable inventory of contributed models and promotes the sharing, reuse, and integration of open-source modeling software. It has adopted a component-based software development model and has created a suite of tools that make the creation of *plug-and-play* components from stand-alone models as automated and effortless as possible. Models or process modules that have been converted to component form are much more flexible and can be rapidly assembled into new configurations to solve a wider variety of scientific problems. The ease with which one component can be replaced by another also makes it easy to experiment with different approaches to providing a particular type of functionality. The CSDMS project also has a mandate from the NSF to provide a migration pathway for surface dynamics modelers toward high-performance computing (HPC) and provides a 720-core supercomputer for use by its members. In addition, CSDMS provides educational infrastructure related to physically based modeling.

The main purpose of this paper is to present in some detail the key issues and design criteria for a component-based, integrated modeling system and then describe the design choices adopted by the CSDMS project to address these criteria. CSDMS was not developed in isolation: it builds on and extends proven, open-source technology. The CSDMS project also maintains

close collaborations with several other integrated modeling projects and seeks to evaluate different approaches in pursuit of those that are optimal. As with any design problem, myriad factors must be considered in determining what is optimal, including how various choices affect users and developers. Other key factors are performance, ease of maintenance, ease of use, flexibility, portability, stability, encapsulation, and future proofing.

1.1. Component Programming Concepts

Component-based programming is all about bringing the advantages of "plug and play" technology into the realm of software. When one buys a new peripheral for a computer, such as a mouse or printer, the goal is to be able to simply plug it into the right kind of port (e.g., a USB, serial, or parallel port) and have it work, right out of the box. For this situation to be possible, however, some kind of published standard is needed that the makers of peripheral devices can design against. For example, most computers have universal serial bus (USB) ports, and the USB standard is well documented. A computer's USB port can always be expected to provide certain capabilities, such as the ability to transmit data at a particular speed and the ability to provide a 5-volt supply of power with a maximum current of 500 mA. The result of this standardization is that one can usually buy a new device, plug it into a computer's USB port, and start using it. Software "plug-ins" work in a similar manner, relying on interfaces (ports) that have well-documented structure or capabilities. In software, as in hardware, the term *component* refers to a unit that delivers a particular type of functionality and that can be "plugged in."

Component programming build on the fundamental concepts of object-

oriented programming, with the main difference being the introduction or presence of a runtime *framework*. Components are generally implemented as classes in an object-oriented language, and are essentially "black boxes" that encapsulate some useful bit of functionality.

The purpose of a framework is to provide an environment in which components can be linked together to form applications. The framework provides a number of *services* that are accessible to all components, such as the linking mechanism itself. Often, a framework will also provide a uniform method of trapping or handling exceptions (i.e., errors), keeping in mind that each component will throw exceptions according to the rules of the language that it is written in. In some frameworks (e.g., CCA's Ccaffeine (Allan et al., 2010)), there is a mechanism by which any component can be promoted to a framework service, as explained in a later section.

One feature that often distinguishes components from ordinary subroutines, software modules, or classes is that they are able to communicate with other components that may be written in a different programming language. This capability is referred to as *language interoperability*. In order for this to be possible, the framework must provide a language interoperability tool that can create the necessary "glue code" between the components. For a CCA-compliant framework, that tool is Babel (Dahlgren et al., 2007; Lawrence Livermore National Laboratory, 2011), and the supported languages are C, C++, Fortran (77-2003), Java, and Python. Babel is described in more detail in a later section. For Microsoft's .NET framework (NET, 2011), that tool is CLR (Common Language Runtime), which is an implementation of an open standard called CLI (Common Language Infrastructure), also developed by

Microsoft. Some of the supported languages are C# (a spin-off of Java), Visual Basic, C++/CLI, IronLisp, IronPython, and IronRuby. CLR runs a form of bytecode called CIL (Common Intermediate Language). Note that CLI does not support Fortran, Java, standard C++, or standard Python.

The Java-based frameworks used by Sun Microsystems are JavaBeans and Enterprise JavaBeans (EJB) (EJB, 2011). In the words of Armstrong et al. (1999):

> Neither JavaBeans nor EJB directly addresses the issue of language interoperability, and therefore neither is appropriate for the scientific computing environment. Both JavaBeans and EJB assume that all components are written in the Java language. Although the Java Native Interface library supports interoperability with C and C++, using the Java virtual machine to mediate communication between components would incur an intolerable performance penalty on every inter-component function call.

While in recent years the performance of Java codes has improved steadily through just-in-time (JIT) compilation into native code, Java is not yet available on key high-performance platforms such as the IBM Blue Gene/L and Blue Gene/P supercomputers.

Key advantages of component-based programming include the following.

- Components can be written in different languages and still communicate (via language interoperability).
- Components can be replaced, added to, or deleted from an application at runtime via dynamic linking (as precompiled units).

- Components can easily be moved to a remote location (different address space) without recompiling other parts of the application (via RMI/RPC support).
- Components can have multiple different interfaces.
- Components can be "stateful"; that is, data encapsulated in the component is retained between method calls over its lifetime.
- Components can be customized at runtime with configuration parameters.
- Components provide a clear specification of inputs needed from other components in the system.
- Components allow multicasting calls that do not need return values (i.e., send data to multiple components simultaneously).
- Components provide clean separation of functionality (for components, this is mandatory vs. optional).
- Components facilitate code reuse and rapid comparison of different implementations.
- Components facilitate efficient cooperation between groups, each doing what it does best.
- Components promote economy of scale through development of community standards.

2. Background

We briefly overview the component methodology used in CSDMS and the associated tools that support component development and application execution.

2.1. The Common Component Architecture

The Common Component Architecture (CCA) (Armstrong et al., 1999) is a *component architecture standard* adopted by federal agencies (largely the Department of Energy and its national laboratories) and academics to allow software components to be combined and integrated for enhanced functionality on high-performance computing systems. The CCA Forum is a grassroots organization that started in 1998 to promote component technology standards (and code reuse) for HPC. CCA defines standards necessary for the interoperation of components developed in different frameworks. Software components that adhere to these standards can be ported with relative ease to another CCA-compliant framework. While a variety of other component architecture standards exist in the commercial sector (e.g., CORBA, COM, .Net, and JavaBeans), CCA was created to fulfill the needs of scientific, high-performance, open-source computing that are unmet by these other standards. For example, scientific software needs full support for complex numbers, dynamically dimensioned multidimensional arrays, Fortran (and other languages), and multiple processor systems. Armstrong et al. (1999) explain the motivation for creating CCA by discussing the pros and cons of other component-based frameworks with regard to scientific, high-performance computing. A number of DOE projects, many associated with

the Scientific Discovery through Advanced Computing (SciDAC) (United States Department of Energy, 2011) program, are devoted to the development of component technology for high-performance computing systems. Several of these are heavily invested in the CCA standard (or are moving toward it) and involve computer scientists and applied mathematicians. Examples include the following.

- TASCS: The Center for Technology for Advanced Scientific Computing Software, which focused on CCA and its associated tools (Bernholdt D. (PI), 2010).
- CASC: Center for Applied Scientific Computing, which is home to CCA's Babel tool (Lawrence Livermore National Laboratory, 2011).
- ITAPS: The Interoperable Technologies for Advanced Petascale Simulation (Diachin L. (PI), 2011), which focuses on meshing and discretization components, formerly TSTT.
- PERI: Performance Engineering Research Institute, which focuses on HPC quality of service and performance issues (Lucas R. (PI), 2011).
- TOPS: Terascale Optimal PDE Solvers, which focuses on PDE solver components (Keyes D. (PI), 2011).
- PETSc: Portable, Extensible Toolkit for Scientific Computation, which focuses on linear and nonlinear PDE solvers for HPC, using MPI (Balay et al., 2010, 2011, 1997).

A variety of different frameworks, such as Ccaffeine (Allan et al., 2010), CCAT/XCAT (Krishnan and Gannon, 2004), SciRUN (de St. Germain et al.,

2002) and Decaf (Kumfert, 2003), adhere to the CCA component architecture standard. A framework can be CCA-compliant and still be tailored to the needs of a particular computing environment. For example, Ccaffeine was designed to support parallel computing, and XCAT was designed to support distributed computing. Decaf (Kumfert, 2003) was designed by the developers of Babel primarily as a means of studying the technical aspects of the CCA standard itself. The important point is that each of these frameworks adheres to the same standard, thus facilitating reuse of a (CCA) component in another computational setting. The key idea is to isolate the components themselves, as much as possible, from the details of the computational environment in which they are deployed. If this is not done, then we fail to achieve one of the main goals of component programming: code reuse.

CCA has been shown to be interoperable with Earth System Modeling Framework (ESMF) (Hill et al., 2004) and Model Coupling Toolkit (MCT) (Larson, 2009; Larson and Norris, 2007; Ong et al., 2008; The MCT Development Team, 2006). CSDMS has also demonstrated that it is interoperable with a Java version of Open Modeling Interface (OpenMI) (The OpenMI Association, 2011). Many of the papers in our cited references have been written by CCA Forum members and are helpful for learning more about CCA. The CCA Forum has also prepared a set of tutorials called "A Hands-On Guide to the Common Component Architecture" (CCA Forum, 2010).

2.2. Language Interoperability with Babel

Babel (Lawrence Livermore National Laboratory, 2011; Dahlgren et al., 2007) is an open-source, language interoperability tool (consisting of a compiler and runtime) that automatically generates the "glue code" necessary

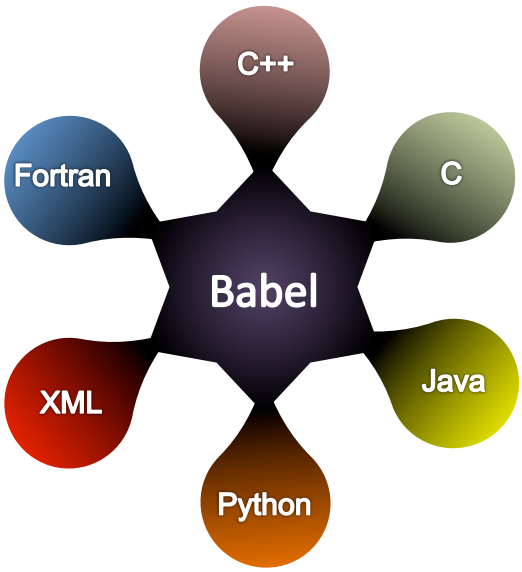


Figure 1: Language interoperability provided by Babel.

for components written in different computer languages to communicate. As illustrated in Fig. 1, Babel currently supports C, C++, Fortran (77, 90, 95, and 2003), Java and Python. Babel is much more than a "least common denominator" solution; it even enables passing of variables with data types that may not normally be supported by the target language (e.g., objects and complex numbers). Babel was designed to support *scientific*, *high-performance* computing and is one of the key tools in the CCA tool chain. It won an R&D 100 design award in 2006 for "The world's most rapid communication among many programming languages in a single application." It has been shown to outperform similar technologies such as CORBA and Microsoft's COM and .NET.

In order to create the glue code needed for two components written in different programming languages to exchange information, Babel needs to

know only about the interfaces of the two components. It does not need any implementation details. Babel was therefore designed so that it can ingest a description of an interface in either of two fairly "language-neutral" forms, XML (eXtensible Markup Language) or SIDL (Scientific Interface Definition Language). The SIDL language (somewhat similar to CORBA's IDL) was developed for the Babel project. Its sole purpose is to provide a concise description of a scientific software component interface. This interface description includes complete information about a component's interface, such as the data types of all arguments and return values for each of the component's methods (or member functions). SIDL has a complete set of fundamental data types to support scientific computing, from Booleans to double-precision complex numbers. It also supports more sophisticated data types such as enumerations, strings, objects, structs,and dynamic multi-dimensional arrays. The syntax of SIDL is similar to that of Java. A complete description of SIDL syntax and grammar can be found in "Appendix B: SIDL Grammar" in the Babel User's Guide (Dahlgren et al., 2007). Complete details on how to represent a SIDL interface in XML are given in "Appendix C: Extensible Markup Language (XML)" of the same guide.

2.3. The Ccaffeine Framework

Ccaffeine (Allan et al., 2010) is the most widely used CCA framework, providing the runtime environment for sequential or parallel components applications. Using Ccaffeine, component-based applications can run on diverse platforms, including laptops, desktops, clusters, and leadership-class supercomputers. Ccaffeine provides some rudimentary MPI communicator services, although individual components are responsible for managing par-

allelism internally (e.g., communicating data to and from other distributed components). A CCA framework provides *services*, which include component instantiation and destruction, connecting and disconnecting of ports, handling of input parameters, and control of MPI communicators. Ccaffeine was designed primarily to support the single-component multiple-data (SCMD) programming style, although it can support multiple-component multiple-data (MCMD) applications that implement more dynamic management of parallel resources. The CCA specification also includes an event service description, but it is not fully implemented in Ccaffeine yet. Multiple interfaces to configuring and executing component applications within the Ccaffeine framework exist, including a simple scripting language, a graphical user interface, and the ability to take over some of the operations normally handled by the frameworks, such as component instantiation and port connections.

A typical CCA component's execution consists of the following steps:

- The framework loads the dynamic library for the component. Static linking options are also available.
- The component is instantiated. The framework calls the `setServices` method on the component, passing a handle to itself as an argument.
- User-specified connections to other components' ports are established by the framework.
- If the component provides a `gov.cca.ports.Go` port (similar to a "main" subroutine), its `go()` method can be invoked to start the main portion of the computation.

- Connections can be made and broken throughout the life of the component.
- All component ports are disconnected, and the framework calls `releaseServices` prior to calling the component's destructor.

The handle to the framework services object, which all CCA components obtain shortly after instantiation, can be used to access various framework services throughout the component's execution. This represents the main difference between a class and a component: a component dynamically accesses another component's functionality through dynamically connecting ports (requiring the presence of a framework), whereas classes in object-oriented languages call methods directly on instances of other classes.

2.4. Component Development with Bocca

Bocca (Allan et al., 2008) is a tool in the CCA tool chain that was designed to help users create, edit, and manage a set of SIDL-based entities, including CCA components and ports, that are associated with a particular project. Once a set of CCA-compliant components and ports has been prepared, one can use a CCA-compliant framework such as Ccaffeine to link components from this set together to create applications or composite models.

Bocca was developed to address usability concerns and reduce the development effort required for implementing multilanguage component applications. Bocca was designed specifically to free users from mundane, time-consuming, low-level tasks so they can focus on the scientific aspects of their

applications. It can be viewed as a development environment tool that allows application developers to perform rapid component prototyping while maintaining robust software- engineering practices suitable to HPC environments. Bocca provides project management and a comprehensive build environment for creating and managing applications composed of CCA components. Bocca operates in a language-agnostic way by automatically invoking the Babel compiler. A set of Bocca commands required to create a component project can be saved as a shell script, so that the project can be rapidly rebuilt, if necessary. Various aspects of an existing component project can also be modified by typing Bocca commands interactively at a Unix command prompt.

While Bocca automatically generates dynamic libraries, a separate tool can be used to create *stand-alone executables* for projects by automatically bundling all required libraries on a given platform. Examples of using Bocca are available in the set of tutorials called "A Hands-On Guide to the Common Component Architecture," written by the CCA Forum members (CCA Forum, 2010).

2.5. Other Component-Based Modeling Projects

We briefly discuss several other component-based projects in the area of Earth system-related modeling.

- The Object Modeling System (OMS) (OMP, 2011) is a pure Java, object-oriented framework for component-based agro-environmental modeling.

- The Open Modeling Interface (OpenMI) (The OpenMI Association,

2011) is an open-source software-component *interface standard* for the computational core of numerical models. Model components that comply with this standard can be configured without programming to exchange data during computation (at runtime). Similar to the CCA component model, the OpenMI standard supports two-way links between components so that the involved models can mutually depend on calculation results from each other. Linked models may run asynchronously with respect to time steps, and data represented on different geometries (grids) can be exchanged by using built-in tools for interpolating in space and time. OpenMI was designed primarily for use on PCs, using either the .NET or Java framework. CSDMS has experimented with OpenMI version 1.4 (version 2.0 was recently released) but currently uses a simpler component interface.

- The Earth System Modeling Framework (ESMF) (ESMF Joint Specification Team, 2011; Hill et al., 2004) is software for building and coupling weather, climate, and related models written in Fortran. ESMF defines data structures, parallel data redistribution, and other utilities to enable the composition of multimodel high-performance simulations.

- The Framework for Risk Analysis of Multi-Media Environmental Systems (FRAMES) (FRAMES, 2011) is developed by the U.S. Environmental Protection Agency to provide models and modeling tools (e.g., data retrieval and analysis) for simulating different environmental processes.

3. Problem Definition – Component-based Plug-and-Play Modeling

Next we discuss the challenges that we faced in tackling the problem of creating plug-and-play modeling capabilities that can be extended and actively used by the CSDMS community.

3.1. Attributes of Earth Surface Process Models

The Earth surface process modeling community has *numerous* models, but it is difficult to couple or reconfigure them to solve new problems. The reason is that they are a heterogeneous set.

- The models are written in *many different languages*, which may be object-oriented or procedural, compiled or interpreted, proprietary or open-source, etc. Languages do not all offer the same data types and features, so special tools are required to create "glue code" necessary to make function calls across the *language barrier*.

- The models typically are not designed to "talk" to each other and do not follow any particular set of conventions.

- The models generally have a *geographic* context and are often used in conjunction with GIS (Geographic Information System) tools.

- The generally consist of one or more arrays (1D, 2D, or 3D) that are being advanced in time according to differential equations or other rules (i.e., we are not modeling molecular dynamics).

- The models use different input and output file formats.

- The models are often *open source*. Even many models that were originally sold commercially are now available as open-source code, for example parts of Delt3D from Deltares and many EDF (Energie du Francais) models.

3.2. Difficulties in Linking Models

Linking together models that were not specifically designed from the outset to be linkable is often surprisingly difficult, and a brute-force approach to the problem often requires a significant investment of time and effort. The main reason is that two models may differ in may ways. The following list of possible differences illustrates this point.

- The models are written in different languages, making conversion time-consuming and error-prone.
- The person doing the linking may not be the author of either model, and the code is often not well-documented or easy to understand.
- Models may have different dimensionality (1D, 2D, or 3D).
- Models may use different types of grids (e.g., rectangles, triangles, and Voronoi cells).
- Each model has its own time loop or "clock."
- The numerical scheme may be either explicit or implicit.

3.3. Design Criteria

The technical goals of a component-based modeling system include the following.

- Support for *multiple operating systems* (especially Linux, Mac OS X, and Windows).

- *Language interoperability* to support code contributions written in procedural languages (e.g., C or Fortran) as well as object-oriented languages (e.g., Java, C++, and Python).

- Support for both *structured and unstructured grids*, requiring a spatial regridding tool.

- *Platform-independent GUIs and graphics* where useful.

- Use of well-established, open-source *software standards* whenever possible (e.g., CCA, SIDL, OGC, MPI, NetCDF, OpenDAP, and XUL).

- Use of *open-source tools* that are mature and have well-established communities, avoiding dependencies on proprietary software whenever possible (e.g., Windows, C#, and Matlab).

- Support for *parallel computation* (multiprocessor, via MPI standard).

- *Interoperability with other coupling frameworks.* Since code reuse is a fundamental tenet of component-based modeling, the effort required to use a component in another framework should be kept to a minimum.

- *Robustness and ease of maintainenance.* It will clearly have many software dependencies, and this software infrastructure will need to be updated on a regular basis.

- Use of *HPC tools and libraries.* If the modeling system runs on HPC architectures, it should strive to use parallel tools and models (e.g., VisIt, PETSc, and the ESMF regridding tool).

- *Familiarity.* Model developers and contributors should not be required to make major changes to how they work.

Expanding the last bullet, developers should not be required to convert to another programming language or use invasive changes to their code (e.g., use specified data structures, libraries, or classes). They should be able to retain "ownership" of the code and make continual improvements to it; someone should be able to componentize future, improved versions with minimal additional effort. The developer will likely want to continue to use the code outside the framework. However, some degree of code refactoring (e.g., breaking code into functions or adding a few new functions) and ensuring that the code compiles with an open-source compiler are considered reasonable requirements. It is also expected that many developers will take advantage of various built-in tools if doing so is straightforward and beneficial.

3.4. Interface vs. Implementation

The word *interface* may be the most overloaded word in computer science. In each case, however, it adheres to the standard, English meaning of the word that has to do with a boundary between two items and what happens at the boundary.

Many people hear the word interface and immediately think of the interface between a human and a computer program, which is typically either

a command-line interfaceor a graphical user interface (GUI). While such interfaces are an interesting and complex subject, this is usually not what computer scientists are talking about. Instead, they tend to be interested in other types of interface, such as the one between a pair of software components, or between a component and a framework, or between a developer and a set of utilities (i.e., an API or a software development kit).

Within the present context of component programming, we are interested primarily in the interfaces between components. In this context, the word *interface* has a specific meaning, essentially the same as in the Java programming language. An interface is a user-defined entity/type, similar to an abstract class. It does not have any data fields, but instead is a named set of methods or member functions, each defined completely with regard to argument types and return types but without any actual implementation. A CCA *port* is simply this type of interface. Interfaces are the name of the game when it comes to the question of reusability or "plug and play." Once an interface has been defined, one can ask the question: Does this component have interface A? To answer the question, we merely have to look at the methods (or member functions) that the component has with regard to their names, argument types, and return types. If a component does have a given interface, then it is said to *expose* or *implement* that interface, meaning that it contains an actual *implementation* for each of those methods. It is fine if the component has additional methods beyond the ones that constitute a particular interface. Thus, it is possible (and frequently useful) for a single component to expose multiple, different interfaces or ports. For example, multiple interfaces may allow a component to be used in a greater variety

of settings. An analogy exists in computer hardware, where a computer or peripheral may actually have a number of different ports (e.g., USB, serial, parallel, and ethernet) to enable it to communicate with a wider variety of other components.

The distinction between *interface* and *implementation* is an important theme in computer science. The word pair *declaration* and *definition* is used in a similar way. A function (or class) declaration tells what the function does (and how to interact with or use it) but not how it works. To see how the function actually works, we need to look at how it has been defined or implemented. C and C++ programmers are familiar with this idea, which is similar to declaring variables, functions, classes, and other data types in a header file with the file name extension .h or .hpp, and then defining their implementations in a separate file with extension .c or .cpp.

Of course, most of the gadgets that we use every day (from iPods to cars) are like this. We need to understand their interfaces in order to use them (and interfaces are often standardized across vendors), but often we have no idea what is happening inside or how they actually work, which may be quite complex.

While the tools in the CCA tool chain are powerful and general, they do not provide a ready interface for linking geoscience models (or any domain-specific models). In CCA terminology, *port* is essentially a synonym for interface and a distinction is made between ports that a given component uses (*uses ports*), and those that it provides (*provides ports*) to other components. Note that this model provides a means of bidirectional information exchange between components, unlike dataflow-based approaches (e.g., OpenMI) that

support unidirectional links between components (i.e., the data produced by one component is consumed by another component).

Each scientific modeling community that wishes to make use of the CCA tools is responsible for designing or selecting component interfaces (or ports) that are best suited to the kinds of models they wish to link together. This is a big job that involves social as well as technical issues and typically requires a significant time investment. In some disciplines, such as molecular biology or fusion research, the models may look quite different from ours. Ours tend to follow the pattern of a 1D, 2D or 3D array of values (often multiple, coupled arrays) advancing in time. However, our models can still be quite different from each other with regard to their dimensionality or the type of computational grid they use (e.g., rectangles, triangles or polygons), or whether they are implicit or explicit in time.

3.5. Granularity

While components may represent any level of granularity, from a simple function to a complete hydrologic model, the optimum level appears to be that of a particular physical process, such as infiltration, evaporation, or snowmelt. At this level of granularity researchers are most often interested in swapping out one method of modeling a process for another. A simpler method of parameterizing a process may apply only to simplified special cases or may be used simply because there is insufficient input data to drive a more complex model. A different numerical method may solve the same governing equations with greater accuracy, stability, or efficiency and may or may not use multiple processors. Even the same method of modeling a given process may exhibit improved performance when coded in a different programming

language. But the physical process level of granularity is also natural for other reasons. Specific physical processes often act within a domain that shares a physically important boundary with other domains (e.g., coastline and ocean-atmosphere), and the fluxes between these domains are often of key interest. In addition, experience shows that this level of granularity corresponds to GUIs and HTML help pages that are more manageable for users.

A judgment call is frequently needed to decide whether a new feature should be provided in a separate component or as a configuration setting in an existing component. For example, a kinematic wave channel-routing component may provide both Manning's formula and the law of the wall as different options to parameterize frictional momentum loss. Each of these options requires its own set of input parameters (e.g., Manning's n or the roughness parameter, z_0). We could even think of frictional momentum loss as a separate physical process, under which we would have a separate Manning's formula and law of the wall components. Usually, the amount of code associated with the option and usability considerations can be used to make these decisions.

Some models are written in such a way that decomposing them into separate process components is not really appropriate, because of some special aspect of the model's design or because decomposition would result in an unacceptable loss of performance (e.g., speed, accuracy, or stability). For example, *multiphysics models*—such as Penn State Integrated Hydrologic Model (PIHM)—represent many physical processes as one large, coupled set of ODEs that are then solved as a matrix problem on a supercomputer.

Other models involve several physical processes that operate in the same domain and are relatively tightly coupled within the governing equations. The Regional Ocean Modeling System (ROMS) is an example of such a model, in which it may not be practical to model processes such as tides, currents, passive scalar transport (e.g., T and S), and sediment transport within separate components. In such cases, however, it may still make sense to wrap the entire model as a component so that it may interact with other models (e.g., an atmospheric model, such as WRF, or a wave model, such as SWAN) or be used to drive another model (e.g., a Lagrangian transport model, such as LTRANS).

4. Designing a Modeling Interface

A component interface is simply a named set of functions (called methods) that have been defined completely in terms of their names, arguments and return values. The purpose of this section is to explain the types of functions that are required and why. The functions that define an interface are somewhat analogous to the buttons on a handheld remote control—they provide a caller with fine-grained control of the model component.

4.1. The "IRF" Interface Functions

Most Earth-science models initialize a set of state variables (often as 1D, 2D, or 3D arrays) and then execute of series of timesteps that advance the variables forward in time according to physical laws (e.g., mass conservation) or some other set of rules. Hence, the underlying source code tends to follow a standard pattern that consists of three main parts. The first part consists of all source code prior to the start of the time loop and serves to set up

or *initialize* the model. The second part consists of all source code *within* the time loop and is the guts of the model where state variables are updated with each time step. The third part consists of all source code after the end of the time loop and serves to tear down or *finalize* the model. Note that root-finding and relaxation algorithms follow a similar pattern even if the iterations do not represent timestepping. A time-independent model can also be thought of as a time-stepping model with a single time step. For maximum plug-and-play flexibility, each of these three parts must be encapsulated in a separate function that is accessible to a caller. It turns out that we get more flexibility if the function for the middle phase is written to accept the start time and end time as arguments.

For lack of a better term, we refer to this Initialize(), Run_Until(), Finalize() pattern as an ***IRF interface***. All of the model coupling projects that we are aware of use this pattern as part of their component interface, including CSDMS, ESMF, OMF, and OpenMI. An IRF interface is also used as part of the Message Passing Interface (MPI) for communication between processes in high-performance computers.

To see how an IRF interface is used when coupling models, consider two models, Models A and B, that do not have this interface. To combine them into a single model, where one uses the output of the other during its time loop, we would need to cut the code from within Model A's time loop and paste it into Model B, or vice versa. The reason is that both models were designed to control the time loop and cannot reliquish this control.

4.1.1. Initialize (Model Setup)

The initialize step puts a model into a valid state that is ready to be executed. Mostly this involves initializing variables or grids that will be used within the execution step. Temporary files that the execution step will read from or write to should also be opened here.

4.1.2. Run_Until (Model Execution)

The run step advances the model from its current state to a future state. For time-independent models the run step simply executes the model calculation and updates the model state so that future calls will not require executing the calculations again. Encapsulating only the code *within* the time loop allows an application to run the model to intermediate states. This is necessary to allow an application to query the model's state for the purposes of (for instance) printing output or passing state data to another model.

4.1.3. Finalize (Model Termination)

The finalize step cleans up after the model is no longer needed. The main purpose of this step to make sure that all resources a model acquired through its life have been freed. Most often this will be freeing allocated memory, but it could also be freeing file or network handles. Following this step, the model should be left in an invalid state such that its run step can no longer be called until it has been initialized again.

4.2. Getter and Setter Interface Functions

A basic IRF interface, while important, really provides only the core functionality of a model coupling interface. A complete interface will also

require functions that enable another component to request data from the component (a getter) or change data values (a setter) in the component. These are typically called within the Initialize() or Run_Until() methods.

4.2.1. Value Getters

Limiting access to the model's state to be through a set of functions allows control of what data the model shares with other programs and how it shares that data. The data may be transferred in two ways. The first is to give the calling program a copy of the data. The second is to give the actual data that is being used by the model (in C, this would mean passing a pointer to a value). The first has the advantage that it hides implementation details of the model from the calling program and limits what the calling program can do to the model. However, the downside of the first method is that communication will be slower (and could be significantly so, depending on the size of the data being transferred).

4.2.2. Value Setters

Variables in a model should be accessed and changed only through interface methods. This approach ensures that users of the interface are not able to change values that the interface implementor does not want them to change. This also detaches the programmer using the interface from the model implementation, thus freeing the model developer to change details of the model without an application programmer having to make any changes.

The setter can also perform tasks other than just setting data. For instance, it might be useful if the setter checked to make sure that the new data is valid. After the setter method sets the data, it should ensure that

the model is still in a valid state.

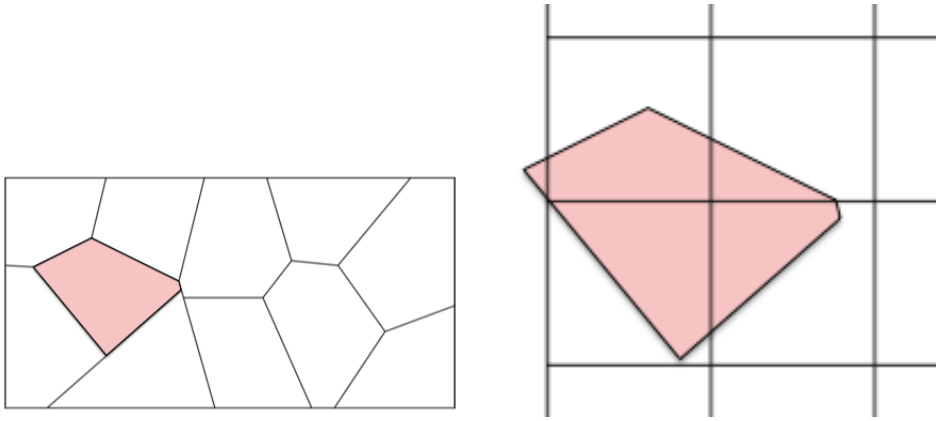
The Get_Value() and Set_Value() methods can be general in terms of supporting different grid or mesh types, but it should be possible to bypass that generality and use simple, raster-based grids to keep things simple and efficient when the generality is not needed.

CSDMS has wrapped two open-source regridding tools that can act as services (see Section 9) that other components can use when communicating with one another (an example regridding scenario is shown in Figure 2). The first is from the ESMF project. It is implemented in Fortran and is designed to use multiple processors on a distributed memory system. It supports sophisticated options such as mass-conservative interpolation. The second tool is the multithreaded tool included in the Java SDK for OpenMI.

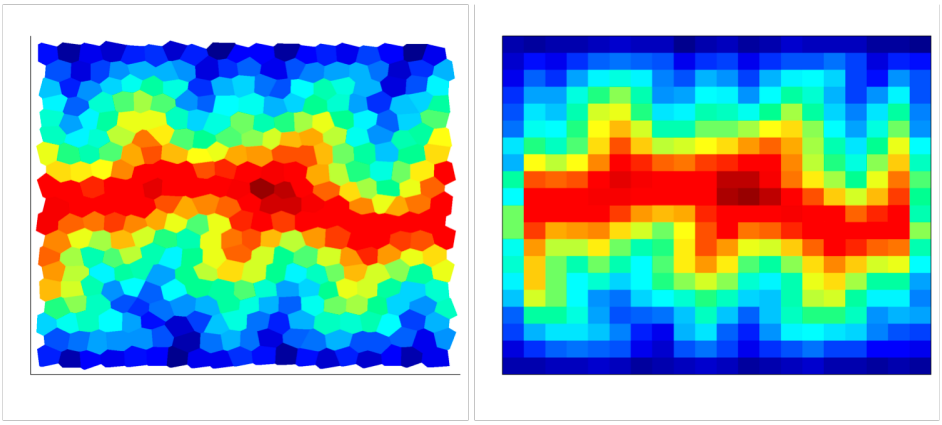
The Get_Value() and Set_Value() methods should optionally allow specification (via indices) of which individual elements within an array that are to be obtained or modified. We often need to manipulate just a few values, and we don'twant to transfer copies of entire arrays (which may be large) unless necessary.

Each component should understand what variables will be requested from it; and if those represent some function of its state variables (e.g., a sum or product), then that computation should be done by the component and offered as an output variable rather than passing several state variables that must then be combined in some way by the caller.

In order to support dynamically typed languages like Python, additional interface functions may be required in order to query whether the variable is currently a scalar or a vector (1D array) or a grid.



(a) Voronoi cells. (b) Intersecting raster and Voronoi cells.



(c) Voronoi cells before regridding. (d) After regridding to raster cells.

Figure 2: Regridding example.

4.3. Self-Descriptive Interface Functions

Two additional methods for a modeling interface would enable a caller to query what type of data the component is able to use as input or compute as output. These would typically not require arguments and would simply return the names of all the possible input or output variables as an array of strings, for example Get_Input_Item_List() and Get_Output_Item_List(). An-

other type of self-descriptive function would be a function like Get_Status() that returns the component's current status as a string from a standardized list.

4.4. Framework Interface Functions

A component typically needs some additional methods that allow it to be instantiated by and communicate with a component-coupling framework. For example, a component must implement methods called __init__(), getServices(), and releaseServices() in order to be used within a CCA-compliant framework.

4.5. Autoconnection Problem

A key goal of component-based modeling is to create a collection of components that can be coupled together to create new and useful composite models. This goal can be achieved by providing every component with the same interface, and this is the approach used by OpenMI. A secondary goal, however, is for the coupling process to be as automatic as possible, that is, to require as little input as possible from users. To achieve this goal, we need some way to group components into categories according to the functionality they provide. This grouping must be readily apparent to both a user and the framework (or system) so that it is clear whether a particular pair of components are *interchangeable*. But what should it mean for two components to be interchangeable? Do they really need to use identical input variables and provide identical output variables? Our experience shows that this definition of interchangeable is unnecessarily strict.

To bring these issues into sharper focus, consider the physical process of infiltration, which plays a key role in hydrologic models. As part of a larger hydrologic model, the main purpose of an infiltration component is to compute the infiltration rate at the surface, because it represents a loss term in the overall hydrologic budget. If the domain of the infiltration component is restricted to the unsaturated zone, above the water table, then it may also need to provide a vertical flow rate at the water table boundary. Thus, the main job of the infiltration component is to provide fluxes at the (top and bottom) boundaries of its domain. To do this job, it needs variables such as flow depth and rainfall rate that are outside its domain and computed by another component. Hydrologists use a variety of different methods and approximations to compute surface infiltration rate. The Richards 3D method, for example, is a more rigorous approach that tracks four state variables throughout the domain; on the other hand, the Green-Ampt method makes a number of simplifying assumptions so that it computes a smaller set of state variables and does not resolve the vertical flow dynamics to the same level of detail (i.e., piston flow, sharp wetting front). As a result, the Richards 3D and Green-Ampt infiltration components use a different set of input variables and provide a different set of output variables. Nevertheless, they both provide the surface infiltration rate as one of their outputs and can therefore be used "interchangeably" in a hydrologic model as an "infiltration component."

The infiltration example illustrates several key points that are transferable to other situations. Often a model, such as a hydrologic model, breaks the larger problem domain into a set of subdomains where one or more pro-

cesses are relevant. The boundaries of these subdomains are often physical interfaces, such as surface/subsurface, unsaturated/saturated zone, atmosphere/ocean, ocean/seafloor, or land/water. Moreover, the variables that are of interest in the larger model often depend on the fluxes across these subdomain boundaries.

Within a group of interchangeable components (e.g., infiltration components), there are many other implementation differences that a modeler may wish to explore, beyond just how a physical process is parameterized. For example, performance and accuracy often depend on the numerical scheme (explicit vs. implicit, order of accuracy, stability), data types used (float vs. double), number of processors (parallel vs. serial), approximations used, the programming language, or coding errors.

Autoconnection of components is important from a user's point of view. Components typically require many input variables and produce many output variables. Users quickly become frustrated when they need to manually create all these pairings/connections, especially when using more than just two or three components at a time. The OpenMI project does not support the concept of auto-connection or interchangeable components. When using the graphical Configuration Editor provided in its SDK, users are presented with droplists of input and output variables and must select the ones to be paired. Doing so requires expertise and is made more difficult because there is so far no ontological or semantic scheme to clarify whether two variable names refer to the same item.

The CSDMS project currently employs an approach to autoconnection that involves providing interfaces (i.e. ,CCA ports) with different names to

reflect their intended use (or interchangeability), even though the interfaces are the same internally.

5. Current CSDMS Component Interface

This section contains a concise list of the current CSDMS IRF and getter/setter interfaces, which must be implemented by any compliant components.

5.1. The IRF Interface

The following methods comprise the IRF interface described in more detail in Section 4.1.

CMI_INITIALIZE (handle, filename)

OUT	handle	handle to the CMI object
IN	filename	path to configuration file

CMI_RUN_UNTIL (handle, stop_time)

IN	handle	handle to the CMI object
IN	stop_time	simulation time to run model until

CMI_FINALIZE (handle)

INOUT	handle	handle to the CMI object

5.2. Value Getters and Setters

The following methods comprise the CSDMS getter/setter interface discussed in Section 4.2.

CMI_GRID_DIMEN (handle, value_str, dimen)

IN	handle	handle to the CMI object
IN	value_str	name of the value to get
OUT	dimen	length of each grid dimension

CMI_GRID_RES (handle, value_str, res)

IN	handle	handle to the CMI object
IN	value_str	name of the value to get
OUT	res	grid spacing for each dimension

CMI_GET_GRID_DOUBLE (handle, value_str, buffer)

IN	handle	handle to the CMI object
IN	value_str	name of the value to get
OUT	buffer	initial address of the destination values

CMI_SET_GRID_DOUBLE (handle, value_str, buffer, dimen)

IN	handle	handle to the CMI object
IN	value_str	name of the value to get
IN	buffer	initial address of the source values
IN	dimen	grid dimension

CMI_GET_TIME_SPAN (handle, span)

IN	handle	handle to the CMI object
OUT	span	start and end times for the simulation

CMI_GET_ELEMENT_SET (handle, value_str, element_set)

IN	handle	handle to the CMI object
IN	value_str	name of the value to get
OUT	buffer	model ElementSet

CMI_GET_VALUE_SET (handle, value_str, value_set)

IN	handle	handle to the CMI object
IN	value_str	name of the value to get
OUT	buffer	model ValueSet

CMI_SET_VALUE_SET (handle, value_str, value_set)

IN	handle	handle to the CMI object
IN	value_str	name of the value to get
IN	buffer	model ValueSet

6. Component Wrapping Issues

In this section we discuss several methods for creating components based on existing codes by using an approach often referred to as *wrapping*.

6.1. Code Reuse and the Case for Wrapping

Using computer models to simulate, predict, and understand Earth surface processes is not a new idea. Many models exist, some of which are fairly sophisticated, comprehensive, and well tested. The difficulty with reusing these models in new contexts or linking them to other models typically has less to do with how they are implemented and more to do with the interface through which they are called (and to some extent, the implementation language.) For a small or simple model, little effort may be needed to rewrite the model in a preferred language and with a particular interface. Rewriting large models, however, is both time-consuming and error prone. In addition, most large models are under continual development, and a rewritten version will not see the benefits of future improvements. Thus, for code reuse to be practical, we need a *language interoperability tool*, so that components dont

need to be converted to a different language, and a *wrapping procedure* that allows us to provide existing code with a new calling interface. As suggested by its name, and the fact that it applies to the "outside" (interface) of a component vs. its "inside" (implementation), wrapping tends to be noninvasive and is a practical way to convert existing models into components.

6.2. Wrapping for Object-Oriented Languages

Component-based programming is essentially object-oriented programming with the addition of a framework. If a model has been written as a class, then it is relatively straightforward to modify the definition of this class so that it exposes a particular model-coupling interface. Specifically, one could add new methods (member functions) that call existing methods, or one could modify the existing methods. Each function in the interface has access to all of the state variables (data members) without passing them explicitly; it also has access to all the other interface functions. In object-oriented languages one commonly distinguishes between *private methods* that are intended for internal use by the model object and *public methods* that are to be used by callers and that may comprise one or more interfaces. (Some languages, like Java, make this part of a method's declaration.)

In order for this model object to be used as a component in a CCA-compliant framework like Ccaffeine, it must also be "wrapped" by a CCA implementation file (or IMPL file). The CCA tool chain has tools such as Babel and Bocca that are used to autogenerate an IMPL-file template. For a model that is written in an object-oriented and Babel-supported language (e.g., C++, Python, or Java), the IMPL file needs to do little more than add interface functions like setServices and releaseServices that allow the

component to communicate with and be instantiated by the framework. The interface functions used for intercomponent communication (i.e., passing data and IRF) can simply be inherited from the model class. Inheritance is a standard mechanism in object-oriented languages that allows one interface (set of methods) to be extended or overridden by another. Note that the IMPL file may have its own Initialize() function that first gets the required CCA ports and then calls the Initialize() function in the model's interface. But the function that gets the CCA ports can simply be another function in the model's interface that is used only in this context. Similarly, the IMPL file may have a Finalize() function that calls the Finalize() function of the model and then calls a function to release the CCA ports that are no longer needed. It is desirable to keep the IMPL files as clean as possible, which means adding some CCA-specific functions to the model's interface. For example, a CSDMS component would have (1) functions to get and release the required CCA ports, (2) a function to create a tabbed-dialog (using CCA's so-called parameter ports), and (3) a function that prints a language-specific traceback to stdout if an exception occurs during a model run.

6.3. Wrapping for Procedural Languages

Languages such as C or Fortran (up to 2003) do not provide object-oriented primitives for encapsulating data and functionality. Because component-based programming requires such encapsulation, the CCA provides a means to produce object-oriented software even in languages that do not support it directly. We briefly describe the mechanism for creating components based on functionality implemented in a procedural language (e.g., an existing li-

brary or model).

A class in object-oriented terminology encapsulates some set of related functions and associated data. To wrap a set of library functions, one can create a SIDL interface or class that contains a set of methods whose implementations call the legacy functions. The new interface does not have to mirror existing functions exactly, presenting a nonintrusive opportunity for redesigning the publicly accessible interfaces presented by legacy software. The creation of class or component wrappers also enables the careful definition of namespaces, thus reducing potential conflicts when integrating with other classes or components. The SIDL definitions are processed by Babel to generate IMPL files in the language of the code being wrapped. The calls to the legacy library can then be added either manually or by a tool, depending on how closely the SIDL interface follows the original library interface.

Function argument types that appear in the SIDL definition can be handled in two ways: by using a SIDL type or by specifying them as *opaque*. SIDL already supports most basic types and different kinds of arrays found in the target languages. Any user-defined types (e.g., structs in C or derived types in Fortran) must have SIDL definitions or be passed as opaques. Because opaques are not accessible from components implemented in a different language, they are rarely used. Model state variables that must be shared among components can be handled in a couple of ways. They can be encapsulated in a SIDL class and accessed through get/set methods (e.g., as described in Section 4.2). Recently Babel has added support for defining *structs* in SIDL, whose data members can be accessed directly from multiple languages.

SIDL supports namespacing of symbols through the definition of packages whose syntax and semantics are similar to Java's packages. In languages that do not support object orientation natively, symbols (e.g., function names) are prefixed with the names of all enclosing packages and parent class. This approach greatly reduces the potential build-, link-, or runtime name conflicts that can result when multiple components define the same interfaces (e.g., the initialize, run, and finalize methods). These naming conventions can be applied to any code, not only SIDL-based components.

Implementors working in non object-oriented languages should encapsulate their model's state data in an object that is opaque to the application programmer. Memory within the object is not directly accessible by the user but can be accessed through an opaque handle, which exists in user space. This handle is passed as the first argument to each of the interface functions so that they can operate on a particular instance of a model. For example, in C, this handle could simply be a pointer to the object and in Fortran, the handle could be an index into a table of opaque objects in a system table.

Model handles are allocated and deallaocated in the initialize and finalize interface functions, respectively. For allocate calls, the initialize functions are passed an OUT argument that will contain a valid reference to the object. For deallocation, the finalize function accepts an INOUT variable that provides a reference to the object to be destroyed and sets the object to an invalid state.

6.4. Guidelines for Model Developers

Developers can follow several relatively simple follow so that it becomes much easier to create a reusable, plug-and-play component from their model

source code. Given the large number of models that are contributed to the CSDMS project, it is much more efficient for model developers to follow these guidelines and thereby "meet us halfway" than for CSDMS staff to make these changes after code has been contributed. This can be thought of as a form of load balancing.

6.4.1. Programming Language and License

- Write code in a Babel-supported language (C, C++, Fortran, Java, Python).
- If code is in Matlab or IDL, use tools like I2PY to convert it to Python. Python (with the numpy, scipy, and matplotlib packages) provides a free work-alike to Matlab with similar performance.
- Make sure that code can be compiled with an open-source compiler (e.g., gcc and gfortran).
- Specify what type of open-source license applies to your code. Rosen (2004) provides a good, online, and open-source book that explains open-source licensing in detail. CSDMS requires that contributions have an open source license type that is compliant with the standard set forth by the Open Source Initiative.

6.4.2. Model Interface

- Refactor the code to have the basic IRF interface (5.1).
- If code is in C or Fortran, add a model name prefix to all interface functions to establish a namespace (e.g., ROMS_Initialize()). C code can alternatively be compiled as C++.

- Write Initialize() and Run_Until() functions that will work whether the component is used as a driver or *nondriver*.
- Provide getter and setter functions (4.2.1).
- Provide functions that describe input and output *exchange items* (4.2.1).
- Use descriptive function names (e.g., Update_This_Variable).
- Remove user interfaces, whether graphical, command line or otherwise, from your interface implementation. This avoids incompatible user interfaces competing with one another.

6.4.3. State Variables

- Decide on an appropriate set of state variables to be maintained by the component and made available to callers.
- Attempt to minimize data transfer between components (as discussed above).
- Use descriptive variable names.
- Carefully track each variable's units.

6.4.4. Input and Output Files

- Do not hardwire configuration settings in the code; read them from a configuration file (text).
- Do not use hardwired input filenames.

- Read configuration settings from text files (often in Initialize()). Do not prompt for command-line input. If a model has a GUI, write code so it can be bypassed; use the GUI to create a configuration file.

- Design code to allow separate input and output directories that are read from the configuration file. This approach allows many users to use the same input data without making copies (e.g., test cases). It is frequently helpful to include a *case prefix* (scenario) and a *site prefix* (geographic name) and use them to construct default output filenames.

- Establish a namespace for configuration files (e.g., ROMS_input.txt vs. input.txt).

- If large arrays are to be stored in files, save them as binary vs. text. (e.g., this is the case with NetCDF)

- Provide self-test functions or unit tests and test data. One self-test could simply be a "sanity check" that uses trivial (perhaps hard-coded) input data. When analytic solutions are available, these make excellent self-tests because they can also be used to check the accuracy and stability of the numerical methods.

- Do not create and write to output files within the interface implementation. If this is not possible, output files should be well documented and allow for a naming convention that reduces the possibility of naming conflicts.

6.4.5. Documentation

- Help CSDMS to provide a standardized, HTML help page.

- Help CSDMS to provide a standaridized, tabbed-dialog GUI.
- Make liberal use of comments in the code.

7. The CSDMS Modeling Tool (CMT)

As explained in Section 2.3, Ccaffeine is a CCA-compliant framework for connecting components to create applications. From a user's point of view, Ccaffeine is a low-level tool that executes a sequence of commands in a Ccaffeine script. The (natural language) commands in the Ccaffeine scripting language are fairly straightforward, so it is not difficult for a programmer to write one of these scripts. For many people, however, using a graphical user interface (GUI) is preferable because they don'thave to learn the syntax of the scripting language. A GUI also provides users with a natural, visual representation of the connected components as boxes with buttons connected by wires. It can also prevent common scripting errors and offer a variety of other convenient features. The CCA Forum developed such a GUI, called Ccafe-GUI, that presented components as boxes in a palette that can be moved into an arena (workspace) and connected by wires. It also allows component configurations and settings to be saved in BLD files and instantly reloaded later. Another key feature of this GUI is that, as a lightweight and platform-independent tool written in Java, it can be installed and used on any computer with Java support to create a Ccaffeine script. This script can then be sent to a remote, possibly high-performance computer for execution.

While the Ccafe-GUI was certainly useful, the CSDMS project realized that it could be improved and extended in numerous ways to make it more powerful and more user-friendly. In addition, these changes would serve not

only the CSDMS community but could be shared back with the CCA community. That is, the new GUI works with any CCA-compliant components, not just CSDMS components. The new version is called CMT (CSDMS Modeling Tool). Significant new features of CMT 1.5 include the following.

- Integration with a powerful visualization tool called VisIt (see below).
- New, "wireless" paradigm for connecting components (see below).
- A login dialog that prompts users for remote server login information.
- Job management tools that are able to submit jobs to processors of a cluster.
- "Launch and go": launch a model run on a remote server and then shut down the GUI (the model continues running remotely).
- New File menu entry: "Import Example Configuration."
- A Help menu with numerous help documents and links to websites.
- Ability to submit bug reports to CSDMS.
- Ability to do file transfers to and from a remote server.
- Help button in tabbed dialogs to launch component-specific HTML help.
- Support for droplists and mouse-over help in tabbed dialogs.
- Support for custom project lists (e.g., projects not yet ready for release).

- A separate "driver palette" above the component palette.
- Support for numerous user preferences, many relating to appearance.
- Extensive cross-platform testing and "bulletproofing."

The CMT provides integrated visualization by using VisIt. VisIt (VisIt, 2011) is an open-source, interactive, parallel visualization and graphical analysis tool for viewing scientific data. It was developed by the U.S. Department of Energy Advanced Simulation and Computing Initiative to visualize and analyze the results of simulations ranging from kilobytes to terabytes. VisIt was designed so that users can install a client version on their PC that works together with a server version installed on a high-performance computer or cluster. The server version uses multiple processors to speed rendering of large data sets and then sends graphical output back to the client version. VisIt supports about five dozen file formats and provides a rich set of visualization features, including the ability to make movies from time-varying databases. The CMT provides help on using VisIt in its Help menu. CSDMS uses a service component to provide other components with the ability to write their output to NetCDF files that can be visualized with VisIt. Output can be 0D, 1D, 2D, or 3D data evolving in time, such as a time series (e.g., a hydrograph), a *profile series* (e.g., a soil moisture profile), a 2D *grid stack* (e.g., water depth), a 3D *cube stack*, or a scatter plot of XYZ triples.

Another innovative feature of CMT 1.5 is that it allows users to toggle between the original, *wired* mode and a new *wireless* mode. CSDMS found that displaying connections between components with the use of wires (i.e., red lines) did not scale well to configurations that contained several compo-

nents with multiple ports. In wireless mode, a component that is dragged from the palette to the arena appears to broadcast what it can provide (i.e., CCA provides ports) to the other components in the arena (using a concentric circle animation). Any components in the arena that need to use that kind of port get automatically linked to the new one; this is indicated through the use of unique, matching colors. In cases where two components in the arena have the same *uses port* but need to be connected to different providers, wires can still be used.

CSDMS continues to make usability improvements to the CMT and used the tool to teach a graduate-level course on surface process modeling at the University of Colorado, Boulder, in 2010. Several features of the CMT make it ideal for teaching, including (1) the ability to save prebuilt component configurations and their settings in BLD files, (2) the File >> Import Example Configuration feature, (3) a standardized HTML help page for each component, (4) a uniform, tabbed-dialog GUI for each component, (5) rapid comparison of different approaches by swapping one component for another, (6) the simple installation procedure, and (7) the ability to use remote resources.

8. Providing Components with a Uniform Help System and GUI

Beyond the usual software engineering definition of a component, a useful component will be one that also comes bundled with metadata that describes the component and the underlying model that it is built around. While creating a component as described in the preceding sections is important, it is of equal importance to have a well-documented component that an end

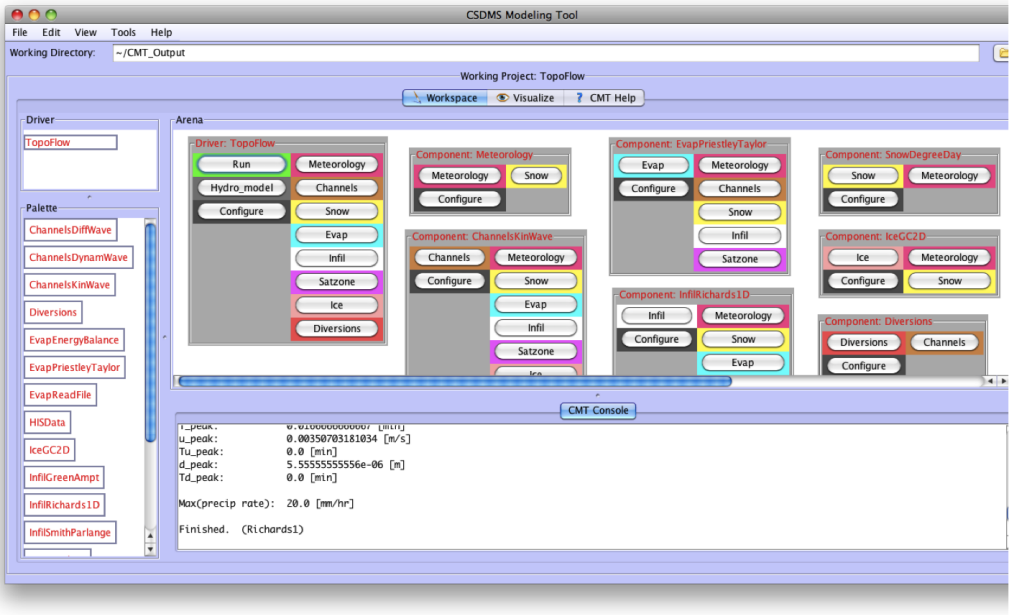


Figure 3: CMT screenshot.

user is able to easily use.

With a plug-and-play framework where users easily connect, interchange, and run coupled models, there is a tendency for a user to treat components as black boxes and ignore the details of the foundation that each component was built upon. For instance, if a user is unaware of the assumptions that underlie a model, that user may couple two components for which coupling does not make sense because of the physics of each model. The user may attempt to use a component in a situation where it was not intended to be used. To combat this problem, components are bundled with HTML help documents, which are easily accessible through the CMT, and describe the component and the model that it wraps. These documents include the following.

- Extended model description (along with references)
- Listing and brief description of the component's uses and provides ports
- Main equations of the model
- Sample input and output
- Acknowledgment of the model developer(s)

A complete component also comes with metadata supplied in a more structured format. Components include XML description files that describe their user-editable input variables. These description files contain a series of XML elements that contain detailed information about each variable including a default value, range of acceptable values, short and long descriptions, units, and data type.

```
<entry name=velocity>
 <label>River velocity</label>
 <help>Depth-averaged velocity at the river mouth</help>
 <default>2</default>
 <type>Float</type>
 <range>
   <min>0</min>
   <max>5</max>
 </range>
 <units>m/s</units>
</entry>
```

Using this XML description, the CMT automatically generates a graphical user interface (in the form of tabbed dialogs) for each CSDMS component. Despite each model's input files being significantly different, this provides CMT users with a uniform interface across all components. Furthermore, the GUI checks user input for errors and provides easily accessible help within the same environment—none of which is available in the batch interface of most models. A special type of CCA *provides port* called a *parameter port* is also used in the creation of the tabbed dialogs.

Nearly every model gathers initial settings from an input file and then runs without user intervention. Ultimately, any user interface that wraps a model must generate this input file for the component to read as part of its initialization step. The above XML description along with a template input file allows this to happen. Once input is gathered from the user, a model-specific input file is created based on a template input file provided with each component. A valid input file is created based on `$`-based substitutions in this template file. Instead of actual values, the template file contains substitution placeholders of the form `$identifier`. Each identifier corresponds to an entry name in the XML description file and, upon substitution, is replaced by the value gathered from an external user interface (the CMT GUI, for instance).

9. Framework Services: "Built-in" Tools That Any Component Can Use

Developers (e.g., CSDMS staff) may wish to make certain low-level tools or utilities available so that any component (or component developer) can use

them without requiring any action from a user. These tools can be encapsulated in special components called *service components* that are automatically instantiated by a CCA framework on startup. The services or methods provided by these components are then called *framework services*. Unlike other components, which users may assemble graphically into larger applications, users do not interact with service components directly. However, a component developer can make calls to the methods of service components through *service ports*. The use of service components allows developers to maintain code for a shared functionality in a single place and to make that functionality available to all components regardless of the language they are written in (or which address space they are in). CSDMS uses service components for tasks such as (1) providing component output variables in a form needed by another component (e.g., spatial regridding, interpolation in time, and unit conversion) and (2) writing component output to a standard format such as NetCDF.

Any CCA component can be "promoted" to a service component. A developer simply needs to add lines to its setServices() method that register it as a framework service. CCA provides a special port for this, *gov.cca.ports.ServiceRegistry*, with three methods: addService(), addSingletonService(), and removeService(). If a developer then wants another component to be able to use this framework service, a call to the gov.cca.Services.getPort() method must be added within its setServices() method. (A similar call must be added in order to use CCA parameter ports and ports provided by other types of components.) Note that the setServices() method is defined as part of the gov.cca.Component interface.

CCA components are designed for use within a CCA-compliant framework (like Ccaffeine) and may make use of service components. But what if we want to use these components outside of a CCA framework? One option is to encapsulate a set of functionality (e.g., a service component) in a SIDL class and then "promote" this class to (SIDL) component status through inheritance and by adding only framework-specific methods like setServices(). (Note that a CCA framework is the entity that calls a component's setServices() method as described in Section 2.3.) This approach can be used to provide both component and noncomponent versions of the class. Compiling the noncomponent version in a Bocca project generates a library file that we can link against or, in the case of Python, a module that we can import.

10. Current Contents of the CSDMS Component Repository

At the time of this publication the CSDMS model repository contains more than 160 models and tools. Of those, 50 have been converted into components as described in this paper and can be used in coupled modeling scenarios with the CMT or through the component composition interfaces supported by Ccaffeine. An up-to-date list is maintained at the CSDMS webiste. As with the model repository as a whole, CSDMS components cover the breadth of surface dynamics systems. Hydrologic components cover various scales ranging from basin-scale (the entire TopoFlow (**?**) suite of models consists of 15 components that cover infiltration, meteorology, and channel dynamics; HydroTrend (**??**)) to reach-scale (the one-dimensional sediment transport models of **?**). Terrestrial components include models of landscape evolution (Erode, and CHILD (**?**)), geodynamics (Subside (**?**))

and cryospherics (GC2D (**?**)). Coastal and marine models include Ashton-Murray Coastal Evolution Model (**??**), Avulsion (**?**), and the stratigraphic model sedflux (**?**). The component repository also contains modeling tools such as the ESMF and OpenMI SDK grid mappers, and file readers and writers for standard file formats (NetCDF, VTK, for example).

11. Conclusions

CSDMS uses a component-based approach to integrated modeling and draws on the combined power of many different open-source tools such as Babel, Bocca, Ccaffeine, the ESMF regridding tool, and the VisIt visualization tool. CSDMS also draws on the combined knowledge and creative effort of a large community of Earth-surface dynamics modelers and computer scientists. Using a variety of tools, standards, and protocols, CSDMS converts a heterogeneous set of open-source, user-contributed models into a suite of plug-and-play modeling components that can be reused in many different contexts. Components that encapsulate a physical process usually represent an optimal level of granularity. Standards that CSDMS has adopted and promotes include CCA, NetCDF (NetCDF, 2011), HTML, OGC (Open Geospatial Consortium) (Open Geospatial Consortium, 2011), MPI (Message Passing Interface) (Message Passing Interface Forum, 1998) and XML (XML, 2011).

All the software that underlies CSDMS is installed and maintained on its high-performance cluster. CSDMS members have accounts on this cluster and access its resources using a lightweight, Java-based client application called the CSDMS Modeling Tool (CMT) that runs on virtually any desktop

or laptop computer. This approach can be thought of as a type of *community cloud* since it provides remote access to numerous resources. This centralized cloud approach offers many advantages including (1) simplified maintenance, (2) more reliable performance, (3) automated backups, (4) remote storage and computation (user's PC remains free), (5) ability for many components (such as ROMS) and tools (such as VisIt and ESMF's regridder) to use parallel computation, (6) requiring to install only a lightweight client on their PC, (7) little technical support needed by users, and (8) ability to submit and run multiple jobs.

Babel's support of the Python language has proven very useful. Python is a modern, open-source, object-oriented language with source code that is easy to write, read and maintain. It runs on virtually any platform. It is useful for system administration, model integration, rapid prototyping, high-level tool development, visualization (via the matplotlib package) and numerical modeling (via the numpy package). Bocca is written in Python, the VisIt visualization package has a powerful Python API, and ESRI's ArcGIS software now uses Python as its scripting language ((Buttler, 2005)). Many third-party geographic information system (GIS) tools implemented in Python are also available. With the numpy, scipy, and matplotlib packages, Python provides a work-alike to commercial languages like Matlab with similar performance. Other Python packages that CSDMS has found useful are *suds* (for SOAP-based web services) and *PyNIO* (an API for working with NetCDF files).

Several exciting opportunities exist for further streamlining and expanding the capabilities of CSDMS. One area of particular interest is how CS-

DMS can provide its members with multiple paths to parallel computation. Software may be designed from the outset to use multiple processors, or be refactored to do so, often using MPI or OpenMP. But this is not easy and typically requires a multiyear investment. Another way to harness the power of parallelism is to modify code to take advantage of numerical toolkits such as PETSc (Portable Extensible Toolkit for Scientific Computation) (Balay et al., 2010, 2011, 1997) that contain parallel solvers for many of the differential equations that are used in physically based models. A third way is to for models written in array-based languages such as IDL, Matlab (MathWorks, 2011) and Python/NumPy (T. Oliphant et al., 2011) to use array-based functions and operators that have been parallelized. This approach, although available only in commercial packages at present, is attractive for several reasons: (1) developers in these languages already know to avoid spatial loops and use the array-based functions whenever possible for good performance, (2) most of these array-based functions are straightforward to parallelize, and (3) developers need only import a different package to take advantage of the parallelized functions.

Web services provide many additional opportunities. Peckham and Goodall (2011) have demonstrated how CSDMS components can use CUAHSI-HIS (CUAHSI, 2011) web services to retrieve hydrologic data, but CSDMS components could also offer their capabilities as web services.

CSDMS is also interested in *automated component wrapping*, which can be achieved by adding special annotation keywords within comments in the source code. If the code is sufficiently annotated, it is possible to write a flexible tool to wrap the component with any desired interface. Unfortunately,

most existing code has not been annotated in this way, and it is typically necessary to involve the code's developer in the annotation process.

Acknowledgments

CSDMS gratefully acknowledges major funding through a cooperative agreement with the National Science Foundation (EAR 0621695). Additional work was supported by the Office of Advanced Scientific Computing Research, Office of Science, U.S. Dept. of Energy, under Contracts DE-AC02-06CH11357 and DE-FC-0206-ER-25774.

References

Allan, B., Armstrong, R., Lefantzi, S., Ray, J., Walsh, E., Wolfe, P., 2010. Ccaffeine – a CCA component framework for parallel computing. `http://www.cca-forum.org/ccafe/`.

Allan, B. A., Norris, B., Elwasif, W. R., Armstrong, R. C., Dec. 2008. Managing scientific software complexity with Bocca and CCA. Scientific Programming 16 (4), 315–327.

Armstrong, R., Gannon, D., Geist, A., Keahey, K., Kohn, S., McInnes, L., Parker, S., Smolinski, B., 1999. Toward a Common Component Architecture for high-performance scientific computing. In: Proc. 8th IEEE Int. Symp. on High Performance Distributed Computing.

Balay, S., Brown, J., , Buschelman, K., Eijkhout, V., Gropp, W. D., Kaushik, D., Knepley, M. G., McInnes, L. C., Smith, B. F., Zhang, H., 2010. PETSc

users manual. Tech. Rep. ANL-95/11 - Revision 3.1, Argonne National Laboratory.

Balay, S., Brown, J., Buschelman, K., Gropp, W. D., Kaushik, D., Knepley, M. G., McInnes, L. C., Smith, B. F., Zhang, H., 2011. PETSc web page. Http://www.mcs.anl.gov/petsc.

Balay, S., Gropp, W. D., McInnes, L. C., Smith, B. F., 1997. Efficient management of parallelism in object oriented numerical software libraries. In: Arge, E., Bruaset, A. M., Langtangen, H. P. (Eds.), Modern Software Tools in Scientific Computing. Birkhäuser Press, pp. 163–202.

Bernholdt D. (PI), 2010. TASCS Center. `http://www.scidac.gov/compsci/TASCS.html`.

Buttler, H., AprilJune 2005. A guide to the python universe for esri users. ArcUser Mag.Available online at `http://www.esri.com/news/arcuser/`.

CCA Forum, 2010. A hands-on guide to the Common Component Architecture. `http://www.cca-forum.org/tutorials/`.

CSDMS, 2011. Community Surface Dynamics Modeling System (CSDMS). `http://csdms.colorado.edu`.

CUAHSI, 2011. Consortium of Universities for the Advancement of the Hydrological Sciences Inc. . `http://www.cuahsi.org`.

Dahlgren, T., Epperly, T., Kumfert, G., Leek, J., 2007. Babel User's Guide. CASC, Lawrence Livermore National Laboratory, UCRL-SM-230026, Livermore, CA.

de St. Germain, J. D., Morris, A., Parker, S. G., Malony, A. D., Shende, S., May 15-17 2002. Integrating performance analysis in the Uintah software development cycle. In: Proceedings of the 4th International Symposium on High Performance Computing (ISHPC-IV). pp. 190–206.
URL http://www.sci.utah.edu/publications/dav00/ishpc2002.pdf

Diachin L. (PI), 2011. Center for Interoperable Technologies for Advanced Petascale Simulations (ITAPS). http://www.scidac.gov/math/ITAPS.html.

EJB, 2011. Enterprise Java Beans Specification. http://java.sun.com/products/ejb/docs.html.

ESMF Joint Specification Team, 2011. Earth System Modeling Framework (ESMF) Website. http://www.earthsystemmodeling.org/.

FRAMES, 2011. Framework for Risk Analysis of Multi-Media Environmental Systems (FRAMES). http://mepas.pnl.gov/FRAMESV1/.

Hill, C., DeLuca, C., Balaji, V., Suarez, M., da Silva, A., ESMF Joint Specification Team, 2004. The architecture of the Earth System Modeling Framework. Computing in Science and Engineering 6, 18–28.

Keyes D. (PI), 2011. Towards Optimal Petascale Simulations (TOPS) Center. http://tops-scidac.org/.

Krishnan, S., Gannon, D., April 2004. XCAT3: A framework for CCA components as OGSA services. In: Proceedings of the 9th International Workshop on High-Level Parallel Programming Models and Supportive Environments (HIPS 2004). IEEE Computer Society, pp. 90–97.

Kumfert, G., April 2003. Understanding the CCA Specification Using Decaf. Lawrence Livermore National Laboratory.
URL http://www.llnl.gov/CASC/components/docs/decaf.pdf

Larson, J. W., 2009. Ten organising principles for coupling in multiphysics and multiscale models. ANZIAM Journal 47, C1090–C1111.

Larson, J. W., Norris, B., 2007. Component specification for parallel coupling infrastructure. In: Gervasi, O., Gavrilova, M. L. (Eds.), Proceedings of the International Conference on Computational Science and its Applications (ICCSA 2007). Vol. 4707 of Lecture Notes in Computer Science. Springer-Verlag, pp. 56–68.

Lawrence Livermore National Laboratory, 2011. Babel. http://www.llnl.gov/CASC/components/babel.html.

Lucas R. (PI), 2011. Performance Engineering Research Institute (PERI). http://www.peri-scidac.org.

MathWorks, 2011. MATLAB - The Language of Technical Computing. http://www.mathworks.com/products/matlab/.

Message Passing Interface Forum, 1998. MPI2: A message passing interface standard. High Performance Computing Applications 12, 1–299.

NET, 2011. Microsoft .NET Framework. http://www.microsoft.com/net/.

NetCDF, 2011. NetCDF. http://www.unidata.ucar.edu/packages/netcdf.

OMP, 2011. Object Modeling System v3.0. http://www.javaforge.com/project/oms.

Ong, E. T., Larson, J. W., Norris, B., Jacob, R. L., Tobis, M., Steder, M., 2008. A multilingual programming model for coupled systems. International Journal for Multiscale Computational Engineering 6, 39–51.

Open Geospatial Consortium, 2011. OGC Standards and Specifications. http://www.opengeospatial.org/.

Peckham, S. D., Goodall, J. L., 2011. Driving plug-and-play components with data from web services: A demonstration of interoperability between CSDMS and CUAHSI-HIS. Computers & Geosciences (this issue).

Rosen, L., 2004. Open Source Licensing: Software Freedom and Intellectual Property Law. Prentice Hall, http://rosenlaw.com/oslbook.htm.

T. Oliphant et al., 2011. Scientific Computing Tools for Python – NumPy. http://numpy.scipy.org/.

The MCT Development Team, 2006. Model Coupling Toolkit (MCT) Web Site. http://www.mcs.anl.gov/mct/.

The OpenMI Association, 2011. The Open Modeling Interface (OpenMI). http://www.openmi.org.

United States Department of Energy, 2011. SciDAC Initiative homepage. http://scidac.gov/.

VisIt, 2011. VisIt. http://wci.llnl.gov/codes/visit.

XML, 2011. Extensible Markup Language (XML). http://www.w3.org/XML/.