

Grid Computing Environments Community Practice (CP) Document

Project Title: Component-Based Problem Solving Environments for Large-Scale Scientific Computing

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Project URL(s): www.sci.utah.edu

1. Overview

SCIRun is a problem solving environment (PSE) that allows the interactive construction, debugging, and steering of large-scale scientific computations. Over the past few years, we have developed two additional problem solving environments that extend SCIRun's capabilities: BioPSE and Uintah. The mission of the BioPSE project is to release state-of-the-art software, datasets, and documentation for researchers investigating bioelectric field problems. Uintah is designed to specifically address the problems of interdisciplinary, massively-parallel scientific computation on terascale computing platforms. These three systems, SCIRun, BioPSE, and Uintah, together target a broad range of vastly different problem domains and application users.

SCIRun provides a component model, based on generalized dataflow programming, that allows different computational components and visualization components to be connected together in a tightly integrated fashion. SCIRun facilitates the interactive construction, debugging and steering of large-scale, typically parallel, scientific computations. SCIRun can be envisioned as a "computational workbench," in which a scientist can design and modify simulations interactively via a component-based visual programming

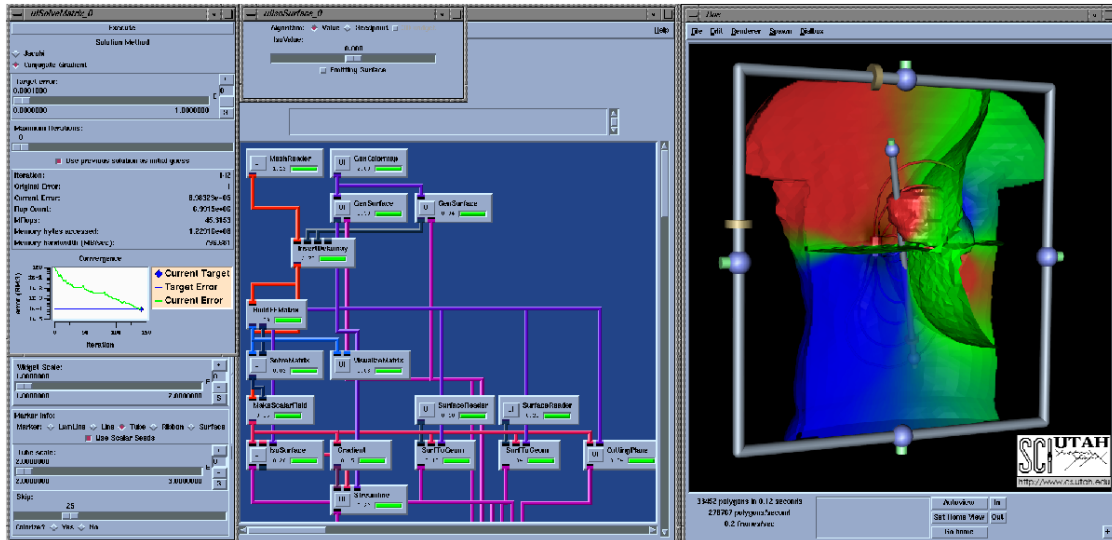


Figure 1. The SCIRun PSE showing the module network (middle), and the visualization window (right). Researchers can select UI (user interaction) buttons on many of the modules that allow control and feedback of parameters within a particular module (left).

model. SCIRun enables scientists to modify geometric models and interactively change numerical parameters and boundary conditions, as well as to modify the level of mesh adaptation needed for an accurate numerical solution. As opposed to the typical “off-line” simulation mode - in which the scientist manually sets input parameters, computes results, visualizes the results via a separate visualization package, and then starts again at the beginning - SCIRun “closes the loop,” allowing interactive steering of the design, computation, and visualization phases of a simulation.

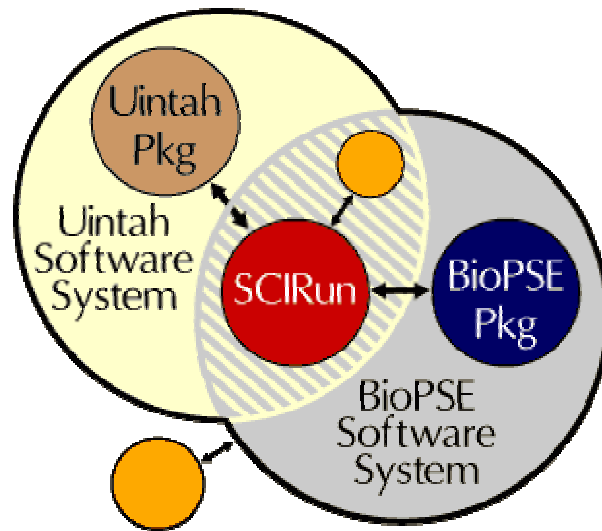


Figure 2. Relationship between the SCIRun, BioPSE, and Uintah software systems.

The BioPSE project seeks to release state-of-the-art software, datasets, and documentation for researchers investigating bioelectric field problems. The immediate applications of this software include forward and inverse bioelectric volume conductor problems, such as localizing electrically active regions of the brain and imaging cardiac activation patterns. We are developing modeling, simulation, and visualization tools that will be of use to researchers engaged in disciplines ranging from cardiac defibrillation device design to cognitive mapping. Our NIH NCCR Center has just begun its third year of funding, and we have just completed our second major software release of the BioPSE system.

Uintah is a Problem-Solving Environment that is being developed to support the University of Utah’s Center for Simulation of Accidental Fires and Explosions (C-SAFE). C-SAFE is funded under the Department of Energy’s Accelerated Strategic Computing Initiative (ASCI) program. The primary goal of C-SAFE focuses specifically on providing state-of-the-art, science-based tools for the numerical simulation of accidental fires and explosions, especially within the context of handling and storage of highly flammable materials. The objective of C-SAFE is to provide a system comprising a problem-solving environment (the Uintah PSE) in which fundamental chemistry and engineering physics are fully coupled with non-linear solvers, optimization, computational steering, visualization and experimental data verification. Uintah extends the capabilities of SCIRun with the addition of the component model being developed by the Department of Energy’s Common Component Architecture (CCA) Forum [1]. While SCIRun and BioPSE currently target shared-memory parallel systems, Uintah uses the CCA component model in a distributed-memory environment for the simulation aspects of the project. Uintah components perform simulations running on hundreds to thousands of processors, computing tens to hundreds of gigabytes of data per simulation.

Each of these software systems are in active use by a wide range of users. SCIRun and BioPSE are publicly available at <http://www.sci.utah.edu>.

2. SCIRun, BioPSE, and Uintah Architectures

SCIRun

The SCIRun architecture [2-4] is the basis for a suite of scientific PSEs that allow the interactive construction, debugging, and steering of large-scale scientific computations. An important feature of the SCIRun architecture enables the user to interactively control scientific simulations while the computation is in progress. This control allows the user, for example, to vary boundary conditions, model geometries, and/or various computational parameters during simulation. Currently, some debugging systems provide similar capability in a low-level form. SCIRun, on the other hand, provides high-level control over parameters in an efficient and intuitive way through graphical user interfaces and scientific visualization. These methods permit the scientist or engineer to “close the loop” and use the visualization to steer phases of the computation.

The ability to steer a large-scale simulation provides many advantages to the scientific programmer. As changes in parameters become more instantaneous, the cause-effect relationships within the simulation become more evident, allowing the scientist to develop more intuition about the effect of problem parameters, to detect program bugs, to develop insight into the operation of an algorithm, or to deepen an understanding of the physics of the problem(s) being studied. The scientific investigation process relies heavily on answers to a range of “what if?” questions. Interaction allows these questions to be answered more efficiently and therefore to guide the investigation as it occurs.

The SCIRun architecture uses a generalized data-flow programming model. A *dataflow network* is assembled by connecting together *modules*, such that each module performs a computational or visualization algorithm. A network is constructed in a visual programming environment that allows for a convenient and natural approach to both application construction and runtime steering. Network data is represented by a set of components, an example of which is the Field class. The Field class provides the ability to adapt data structures from an external simulation to SCIRun’s visualization components and many of the computational components. Uintah, described below, seeks to expand on the success of the component-based approach, by providing a component model based on the DOE Common Component Architecture, a model which is more familiar to programmers who have used the Object Management Group’s (OMG) CORBA [11], or Microsoft’s COM [12].

Initially, we designed SCIRun to solve specific problems in Computational Medicine, but we have since made extensive efforts to make the SCIRun architecture applicable in other computational science and engineering problem domains [5]. In addressing specific problems, we found that there are a wide range of disparate demands placed on a steerable problem solving environment such as the SCIRun system. To meet these demands, we have extended SCIRun with the constructs of *Packages* and *bridging*, and when appropriate, we have even produced derived systems, such as *BioPSE* and *Uintah*. These relationships are depicted graphically in Figure 2, and are further described in the BioPSE and Uintah sections.

Parallelism in SCIRun

SCIRun utilizes two methods of parallelism. The first, task parallelism, is implemented automatically by simultaneously executing multiple modules according to the dataflow graph. Since task parallelism is very limited in the typical scientific application, the second method of parallelism is to explicitly parallelize various modules in a data-parallel (SPMD) fashion. A set of worker threads will be mapped to various processors and will cooperate in accomplishing the function of the module. The worker threads may use the synchronization primitives provided by the Multitask library to communicate with one another.

The shared memory assumption allows for a simple, clean implementation of steerable parameters with low synchronization overhead in the normally running cases. As an example of parallelism, a simple data-parallel conjugate gradient matrix solver in SCIRun achieves a 90% parallel efficiency on 16 MIPS R10K (195 Mhz) processors, solving a 200,000 row sparse matrix with 3.2 million non-zeros in 32 seconds.

Components of SCIRun

In order to implement a steerable application, we have broken down SCIRun into a layered set of libraries. SCIRun uses an object-oriented design; however, it should be stressed that we have paid careful attention to avoid over-using the object-oriented paradigm to a point that efficiency suffers. In implementing the SCIRun kernel and modules, we leverage off of a powerful toolbox of C++ classes that have been tuned for scientific computing and operation in a multi-threaded environment.

SCIRun derives much of its flexibility from its internal use of threads. Threads allow multiple concurrent execution paths in a single program. SCIRun uses threads to facilitate parallel execution, to allow user interaction while computation is in progress, and to allow the system to change variables without interrupting a simulation. However, standards for implementing threads are only starting to appear, and the standards that are appearing are, thus far, cumbersome. We have constructed a layer that provides a simple, clean C++ interface to threads and provides abstraction from the actual standard used to implement them (currently pthreads and SGI sproc).

Data Structure Management

Many implementations of the dataflow paradigm use the port/connection structure to make copies of the data. Consider the example in Figure 3. If the vector field is copied to both the Hedgehog and Streamline visualization modules, then twice as much memory is consumed as necessary. In addition, a significant amount of CPU time is required to copy large, complex data structures. To avoid these overheads, we employ a simple reference counting scheme with *smart pointers* in C++. This scheme helps reduce complexity by allowing different modules to share common data structures with copy-on-write semantics. When the Gradient module creates the VectorField, it sets a reference count in the vector field to zero. As Gradient hands a copy of the vector field data structure to each of the downstream modules, the receiving module increments the reference count. When each module is finished with the data structure, it decrements the reference count. When the reference count reaches zero, the object is destroyed. These reference counts are maintained automatically by C++ classes (the smart pointers) to reduce programmer error. Copying the object is necessary only when a module needs to change a data structure and the reference count is greater than one (i.e., another module is also using it).

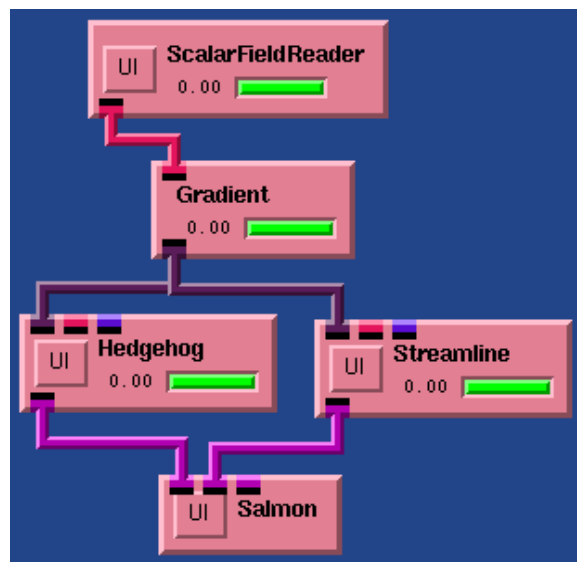


Figure 3. A close-up view of a SCIRun dataflow network. Both the Streamline and Hedgehog modules consume a vector field produced by the Gradient module. In SCIRun, the data are shared between the modules so that the data do not need to be duplicated.

Progressive Refinement and Exploiting Coherence

Due to memory and speed limitations of current computing technologies, it will not always be possible to complete these large-scale computations at an interactive rate. To maintain some degree of dynamic interactivity, the system displays intermediate results as soon as they are available. Such results include partially converged iterative matrix solutions, partially adapted finite element grids, and incomplete streamline or isosurface visualizations.

A common interactive change consists of moving and orienting portions of the geometry. Because of the nature of this interaction, surface movement is apt to be restricted to a small region of the domain. Using information about how the geometry has moved and its position prior to the move, the system can anticipate results and “jump start” many of the iterative methods. For example, iterative matrix solvers can be jump-started by interpolating the solution from the old geometry onto the new mesh. When changes to the model geometry are small, the resulting initial guess is close to the desired solution so the solver converges rapidly. This concept is similar to exploiting temporal coherence in a time-dependent system by using the previous time-step as the initial guess to the next time step. An even more compelling example is seen in the mesh generation. Typically, mesh generation for large-scale geometric models can take tens of minutes to hours to compute. Since it is sometimes the case that users only want to try a slight modification of the geometry or a new location for sources, they can modify and update the mesh only in those places where it is needed in a short amount of time.

For most boundary value and initial value problems, the final answers will be the same for the incremental and brute-force approaches (subject to numerical tolerances). However, for nonlinear problems where there may be multiple solutions or for some unsteady problems, results may be completely different. In these instances, the interaction coherence should not be exploited or results will not be scientifically repeatable.

Through coupling each of these techniques, we are able to introduce some degree of interactivity into a process that formerly took hours, days or even weeks. Although some of these techniques (such as displaying intermediate results) add to the computation time of the process, we attempt to compensate by providing optimizations (such as exploiting interaction coherence) that are not available with the old “data file” paradigm.

Steering and Interaction in a Dataflow System

The dataflow mechanism and the modules have been designed to support steering of large-scale scientific simulations. SCIRun uses three different methods to implement steering in this dataflow-oriented system:

- **Direct lightweight parameter changes:** A variable is connected to a user interface widget, and that variable is changed directly (by another thread) in the module. As an example, the iterative matrix solver module allows the user to change the target error even while the module is executing. This parameter change does not pass a new token through the dataflow network but simply changes the internal state of the SolveMatrix module, effectively changing the definition of the operator rather than triggering a new dataflow event.
- **Cancellation:** When parameters are changed, the module can choose to cancel the current operation. For example, if boundary conditions are changed, it may make sense to cancel the computation to focus on the new solution. This might make sense, for example when solving problem governed by an elliptic partial differential equation, since the solution does not depend on any previous solution.
- **Feedback loops in the dataflow program:** For a time varying problem, the program usually goes through a time stepping loop with several major operations inside. The boundary conditions are integrated in one or more of these operations. If this loop is implemented in the dataflow system, then the user can make operator changes that are integrated on the next trip through the loop.

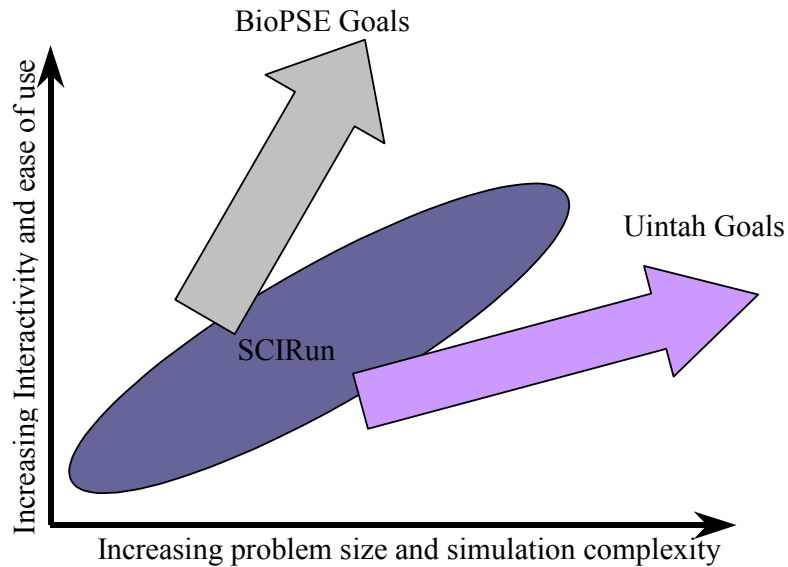


Figure 4. The SCIRun core provides a collection of general utility data types, modules, and services. The BioPSE system targets less experienced programming end users, and as such has focused on extending SCIRun with easy-to-use development tools, and simplified user interfaces. In contrast, Uintah is intended for terascale simulations of extremely complex systems, and has accordingly extended SCIRun with component-based distributed computing and large-scale workflow scheduling capabilities to meet those needs.

BioPSE

The BioPSE system is built on top of the SCIRun core architecture. With each release, we have improved the underlying SCIRun core and added support for a growing number of bioelectric field research problems. The BioPSE package (that part which is additional to SCIRun) consists of new modules and data-structures that are specifically customized for bioelectric volume conductor problems. These pieces include modules for bioelectric field finite element approximation, boundary condition assignment, and inverse source localization. While the bioelectric field modules are significant, they only represent a small percentage of the BioPSE project effort. The major undertaking of the BioPSE project has been to apply solid software engineering approaches to make the SCIRun code and underlying software architecture more robust. Through this process, we have redesigned and extended much of the SCIRun core. Some of these enhancements are described below.

Bridging is one of the newer design pillars of the SCIRun architecture. Philosophically, we have always believed that SCIRun would be most powerful and most useful if it supported flexible mechanisms for the importing and exporting of data and services. To date, we have introduced three levels of bridging. These bridges vary in how tightly they integrate the third party functionality. The tightest level of integration is what we call “assimilation bridging”: we simply rewrite the existing data or functionality within the SCIRun system. This approach is the most time-intensive, and is demonstrated in our Focusing Inversion research project [6], where we have converted MATLAB code into C++ and embedded it within SCIRun. The second level is “library bridging”: we make calls into third party libraries or wrap up third party data structures, and use their functionality within SCIRun modules. An example of library bridging has been to use the grid enabled Netsolve package for solving linear systems from SCIRun. We linked in the Netsolve client libraries and added support for invoking various Netsolve preconditioners and solvers to SCIRun [7]. The third level of bridging is “I/O bridging”: we exchange data through files, sockets, or databases, and invoke external functionality through system calls. We have used I/O bridging with MATLAB, where we communicate via sockets and with a third-party database package to exchange data between SCIRun and

MATLAB. We have also used it extensively in our development of filters for importing/exporting data between SCIRun and other systems.

A major piece of software infrastructure work has been the improvement of the interface to the templated Fields classes. Fields are used to represent geometric domains and data values over that domain. The design challenge for Fields has been to create completely general and flexible data structures, without sacrificing system performance. This requirement is challenging because in order to support a general interface the calling code cannot know in advance what type of Fields will be passed as input, and therefore the code is impossible to optimize in advance. To circumvent this drawback, we designed an easy to use mechanism known as “dynamic compilation and loading” (DCL). The way this mechanism works is that as soon as a module finds out which specific type of Fields have been passed to it as input, it begins compiling optimized code for that specific case; when the code is compiled, this system loads that library and executes it. All of this happens transparently to the user, and has been designed to be simple to use for developers. The advantage to this technique is that we only generate specific optimized code for the types of fields in which we are interested.

BioPSE and the underlying SCIRun core have matured significantly through the development efforts of the NCCR Center. We presently have dozens of users, and anticipate that number will rise rapidly as we continue to add bioelectric field and infrastructure functionality. Enhancing the SCIRun core will continue to be a priority of the NCCR project for the foreseeable future.

For bioelectric field simulations, we will be adding transient visualization methods, and a growing array of inverse techniques. And we will continue adding surface and volume mesh generation tools into the system. In terms of general enhancements to the SCIRun architecture, we will first be designing and implementing state and event management tools. These will serve as stepping stones for our subsequent development of collaborative computing, scripting, and checkpointing capabilities. We will also be implementing multi-resolution modeling, simulation, and visualization techniques that we believe will be of general use to researchers working with large-scale data.

Uintah

C-SAFE was created by the Department of Energy's (DOE) Accelerated Strategic Computing Initiative's (ASCI) Academic Strategic Alliance Program (ASAP). The purpose of ASAP is to “engage the best minds in the U.S. academic community to help accelerate the emergence of new unclassified simulation science and methodology and associated supporting technology for high-performance computer modeling and simulation” [<http://www.llnl.gov/asci-alliances>]. C-SAFE, located on the University of Utah campus, “is focused on providing state-of-the-art, science-based tools for the numerical simulation of accidental fires and explosions.” [C-SAFE Annual Report, Year2, p2] C-SAFE is staffed by twenty key University of Utah faculty, faculty from BYU and WPI, experimental scientists from Thiokol, eighteen post doctoral/professionals, and 14 graduate students. These personnel are divided into six teams: Fire Spread, Container Dynamics, High Energy Transformations, Applied Math, Computer Science, and Validation. It is the combined strengths of these assorted disciplines that are allowing C-SAFE to create a software system that will accurately model the physical processes in our simulations while taking advantage of massively parallel computers to solve the problems in a reasonable amount of time.

Within C-SAFE, it is the Computer Science team's task to architect and implement a software system that will provide the ability to run large multi-physics simulations on massively parallel computers. To fulfill this mission, we are in the process of designing and implementing the Uintah PSE. Uintah is based upon the SCIRun PSE architecture, utilizing the visual dataflow programming paradigm. It has helped extend the SCIRun architecture in two important manners: Uintah has added the Common Component Architecture's (CCA) interchangeable component programming model to SCIRun, and Uintah has added support for running under a mixed shared memory/message passing model [8]. These additions to SCIRun have paved the way in making Uintah a scalable, high-performance system that is capable of solving large scale, very complex scientific problems.

C-SAFE has set a number of ambitious software goals that are intended to push the envelope of large-scale scientific computing. In order to accomplish the extremely complex goal of accurately simulating a large-scale fire engulfing complex materials, the simulation must take into account processes ranging from the atomic level to tens of meters, and time steps from seconds down to femtoseconds. This process is an active collaboration between chemists, mechanical engineers, chemical engineers, and computer scientists; each playing an important and necessary role in creating a unified simulation system. The C-SAFE system, named Uintah, is comprised of a number of software pieces: Blazer (a Scientific Data Management System), Uintah PSE (discussed in detail in this paper), and independent applications that produce the necessary data for the Uintah PSE to accurately perform the simulations.

An important criteria for creating a software system that will effectively utilize large numbers of CPUs working in concert is the development of a parallelization strategy that encompasses both shared memory and MPI style message passing, allowing PSE based simulations to run on a number of different computer architectures.

Another important criterion taken into account in the design of the Uintah PSE is the ability to remotely create and monitor simulations on large, geographically remote, super computers. Grid services, such as remote communication and authentication are essential for these features. While these features are still under development, we are currently using the Globus toolkit to develop these services.

A third criterion driving the design of the Uintah PSE is the ability to easily allow users to investigate the effect of different routines on a simulation and to integrate other software sub-systems into the PSE. This ability is provided by adhering to the Common Component Architecture model being developed by a consortium of National Lab, Industry, and Academic scientists. When complete, this technology will raise the bar from code reuse, to working component reuse.

The current trend in super computing is to use a large number of full-function processors, grouped in shared memory nodes of 2 to 128 processors. These nodes communicate with each other using high speed data interconnects. To take full advantage of this type of architecture, processes running on a single node must take advantage of the benefits of shared memory to reduce communication overhead and problem complexity.

3. Implementation

The combination of SCIRun, Uintah, and BioPSE consist of over 500,000 lines of C++ code. In addition, the user interface is written in Tcl/Tk, and various components use C and Fortran code. XML is used throughout, for describing components to the SCIRun scheduler, and for representing data input and output in Uintah. In addition, we rely on a whole host of commodity software, such as PETSc [13] from Argonne National Laboratory, LAPACK [14], BLAS [15], OpenGL from SGI, pthreads from Posix, Apache's Xerces XML toolkit [16], GNU autoconf., GNU make, and Tuning and Analysis Utilities (TAU) [18] from the University of Oregon.

The core of Uintah is centered around the DOE Common Component Architecture component model. The CCA specification is still evolving but Uintah uses CCA components to implement different aspects of the simulation. Example components are Computational Fluid Dynamics models, Solid Modeling models, Chemical Reaction models, Parallel schedulers, and load balancers.

As previously mentioned, SCIRun and BioPSE are currently publicly available as open-source software. We intend to make Uintah available in the same manner at some point in the future. As much as possible these systems are built on public standards, leveraging existing third party software.

4. Supported Grid Services

SCIRun and its derivatives are currently moving from a standalone program to a more distributed programming model. This transition involves adapting grid services to perform many functions that programmers take for granted on a single shared-memory parallel machine.

As a first step towards incorporating remote visualization to SCIRun we have added a remote image-based rendering (IBR) viewer to the system. By using view dependent isosurfacing [17] and resampled meshes (from a mesh derived from a simplified depth buffer and image buffer) we are able to obtain favorable frame rates with low latency in a variety of grid environments. The client-side viewer has been written in Java with platform independence in mind.

SCIRun, as with most problem solving environments, has a great potential to benefit from most of the services offered by the grid. To date, we have utilized many grid services in different aspects of the implementation. SCIRun has used Netsolve [7,8,10] to provide a mechanism for distributing linear algebra components. Uintah utilizes Nexus (now called Globus I/O), a part of the Globus toolkit [10], to provide inter-component communication for distributed-memory components. Uintah provides Blazer a mechanism for indexing and managing large datasets via the world-wide web.

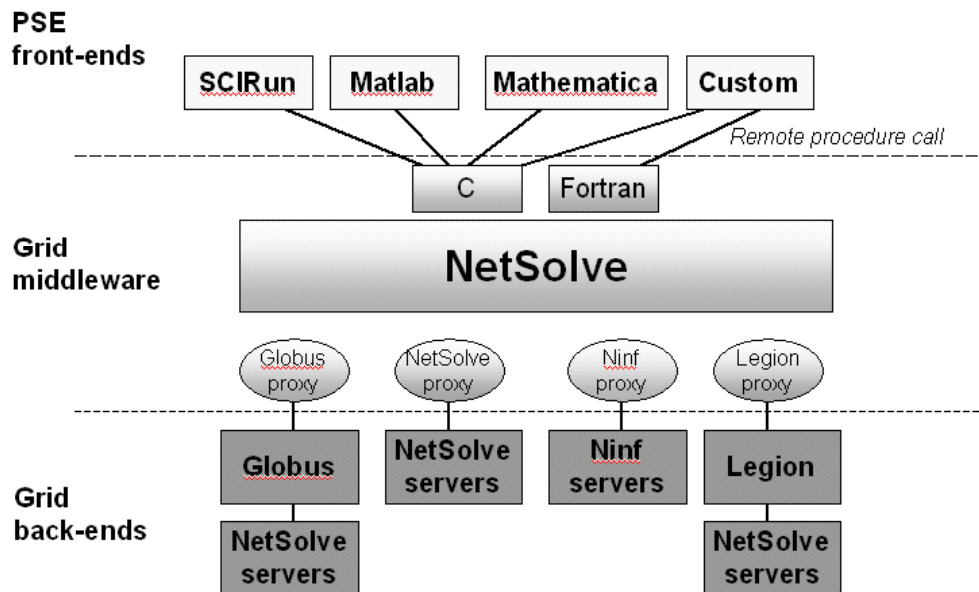


Figure 5. The relationship between application problem solving environments, such as SCIRun, Grid middleware, such as NetSolve, and Grid back-ends.

Other ongoing projects in SCIRun, Uintah, and BioPSE are considering the use of grid services for other applications. Uintah would benefit from the security and scheduling capabilities to implement component staging and scheduling. BioPSE is examining possibilities to utilize microscopes, magnetic resonance machines, and other large-scale instruments via the web.

As problem solving environments become more comprehensive, more distributed, and undoubtedly more complex, grid services become an essential part of the system. Standardization and wide-spread adoption of these services continue to be the key ingredients for successful application of grid services in a PSE.

However, we note that many high level applications are not readily able to utilize grid services because of the significant difficulty in integrating grid services with complex applications. There seems to be a “gap” between low-level grid services and large-scale user applications and front ends. It seems to us that there needs to be a significant, coordinated effort in creating software tools that allow application programs to more easily take advantage of grid services. As we have recently created a “module maker” that helps enable users to import their own codes within SCIRun and BioPSE, we could envision a similar software tool for helping users import and integrate grid software tools within application codes.

5. Project Status and Future Plans

SCIRun, BioPSE, and Uintah are all long-term development projects that support a wide variety of research. Many of the ongoing research projects will require further integration of grid computing services.

Some of the key aspects include:

- Completion of the CCA-based component model: This will include support for component staging, management of available resources, and parallel-to-parallel component communication. In addition, we are working to separate the SCIRun graphical user interface, and will use it to provide visual programming capabilities for a number of different applications.
- Implementation of simulation components for clusters: Clusters are becoming a popular mechanism for providing inexpensive computing cycles. In addition to the efforts underway in Uintah to provide mechanisms for large distributed-memory supercomputers, BioPSE intends to provide components that will utilize small to medium clusters of inexpensive personal computers.
- Remote visualization: Often, the computing resources used to perform a simulation are not located physically near the scientists. In order to view the data, the scientist transports the data to his/her desktop workstation or local visualization workstation. However, datasets often overwhelm local resources. We are attempting to bridge this distance gap and are developing components for generating visualizations on remote computing resources, and using advanced methods in computer graphics to transmit those visualizations back to a remotely located desktop workstation in an interactive manner.
- Cluster-based visualization: In the same manner that Beowulf clusters have revolutionized simulation by providing low-cost mechanisms for obtaining computing cycles, we expect that the same revolution to apply to visualization capabilities using commodity 3D video cards. However, the software required to harness the power of multiple video cards is not mature. We have several ongoing projects that are developing components for cluster-based parallel computer graphics.

We look forward to working with the grid services community to help develop software systems that can benefit computational science and engineering end users.

6. Acknowledgments

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