

Simulation Factory: Taming Application Configuration and Workflow on High-End Resources

Michael W. Thomas

Center for Computation & Technology/
Department of Computer Science
Louisiana State University

Erik Schnetter

Center for Computation & Technology/
Department of Physics & Astronomy
Louisiana State University

Abstract—Computational Science on large high performance computing resources is hampered by the complexity of these systems. Much of this complexity is due to low-level details on these resources that are exposed to the application and the end user. This includes (but is not limited to) mechanisms for remote access, configuring and building applications from source code, and managing simulations and their output files via batch queue systems.

These challenges multiply in a modern research environment, where a research collaboration spans multiple groups, often in loosely defined international collaborations, where there is a constant influx of new students into multi-year projects, and where simulations are performed on several different resources.

The *Simulation Factory* addresses these challenges by significantly simplifying remote access, building executables, and managing simulations. By abstracting out the low-level differences between different resources, it offers a uniform interface to these resources. At the same time, it can enforce certain standards for performing simulations that encapsulate best practices from experienced users. Furthermore, SimFactory’s automation avoids many possible user errors that can in the worst case render month-long simulations worthless.

The Simulation Factory is freely available under an open source license.

I. INTRODUCTION

Although the speed and performance of high end computers have increased dramatically over the last decade, the ease of using such parallel computers has not progressed. The time and effort required to develop and deploy parallel codes and to manage and post-process simulations has become a bottleneck in many areas of science and engineering. The difficulty of using high performance computing is recognized as one of the most significant challenges today in many areas of science and engineering. Simplifying this is crucial to expanding the understanding in these fields via the use of high performance computing.

To simplify code development, large software projects use a modular design or may employ software frameworks. These aid in handling different versions, managing many users, distributed code development, and complex machine architectures. *Cactus* [1], [2] is one such software framework for science applications which is used to simulate physical systems in different fields of science such as black holes

and neutron stars in general relativity. As in other software frameworks, applications are built from separately developed and tested components.

To effectively begin using high performance computing (HPC), one has to overcome a set of unique technical challenges which have their roots in the fact that HPC systems are expensive and unique, very different from commodity workstations. These challenges include:

- *preventing lock-in*: the fundamental need to use multiple HPC systems, since individual systems may be unavailable at any given time, and since HPC systems have a much shorter life time than software;
- *lack of standards*: the fact that each HPC system is often designed independently and can have very different hardware architectures and usage policies;
- *expensive mistakes*: the low-level interface that HPC systems offer to manage simulations which require batch submissions and frequent maintenance of ongoing simulations with dire consequences for user errors that can destroy weeks of data. For example, a job may accidentally be started in the wrong directory and then overwrite existing data, or data may accidentally be deleted before they are successfully archived. Such errors happen “naturally” if a user has to manually manage several jobs at the same time.

For example, HPC systems differ in the available software and their versions, their directory structure and file systems, queuing systems, and policies, in addition to their hardware differences. This makes porting codes, handling data, and setting up simulations very tedious tasks on each system anew. Yet for scientific results none of these differences actually matter. Because HPC systems have a relatively small number of users compared to commodity systems, there is no obvious economic motivation to improve the situation, since most heavy users of HPC systems have already become adept at handling these differences. At the same time, large HPC centers compete for funding (e.g. the 11 sites providing TeraGrid resources for NSF) and for users. They thus have to ensure they stand out and don’t merely copy another centre’s

practice. This makes standardization difficult.

Due to these challenges, users typically adopt one of two modes of operation: one, where one decides on one particular version of the software and one HPC system, and then uses these exclusively, and another, where one leaves these details to graduate students who then have to spend a significant amount of time with these frustrating low-level details. These challenges also lead to the perception that high performance computing is very difficult and hinders update by newcomers.

To help drive forward a broader vision of HPC, we argue that handling these details should not be the responsibility of users in the first place, but should rather be folded into the actual systems. We introduce the *Simulation Factory*, a high-level interface to managing source code, accessing remote systems, and performing simulations. The Simulation Factory, also known as *SimFactory*, offers an abstract work flow covering these tasks and offers a small set of commands for the most-often required actions. All system details are described in a *machine database*. Thus, the Simulation Factory offers a uniform interface to users and renders different HPC system into fungible¹ resources.

A. Related Work

Many component frameworks face problems of collecting components from various independent sources. The Eclipse [3] approach is probably most similar to the one we describe below, with the exception that installing or updating Eclipse components requires Eclipse (and a graphical user interface) to be running, which can be inconvenient or prohibitive on HPC systems. Eclipse also automatically enforces dependencies between different versions of components; this is convenient or necessary for a framework where most users are only end-users, but probably inconvenient for a scenario where most users are also developers and modify code so that the concept of a “version” with a well-defined API is not well defined.

UBIQIS (ubiquitous install) [4] is a system for automatically fetching and installing software from the web or even a peer to peer network. It provides a place from where one can automatically get software, but it does not require root permissions to install, and the software repository is not centralized. It automatically caches requests for software, automatically fetching dependencies as they are needed. We are exploring in how far UBIQIS can be incorporated into the Simulation Factory [5].

Since its first release, Cactus has included a mechanism for groups or individuals to maintain their own set of configuration files for compiling their particular applications. A default set of files was also distributed along side Cactus which were sufficient to build the complete set of distributed thorns on machines supported by the Cactus group with different option files provided for different purposes (e.g. single processor, MPI, debug). Since these option files followed a particular naming convention and were available anonymously via CVS they could be included in higher level tools for Cactus.

For automated configuring and building, we describe and compare to related approaches in section III-B, where we also discuss the requirements that these have to satisfy.

An early driver for automated processes for compilation and run time support came from Cactus’ role in the development and prototyping of Grid Computing scenarios for scientific computing. For example, in 2002 and 2003, a set of tools (dubbed “GridTools” [6], and written in Perl) was developed by Ian Kelley that acted as a compilation, deployment, testing and prototyping infrastructure for Cactus on top of the Globus Toolkit [7] command-line tools, which are a set of tools for grid computing that provide authentication, file transfer, job submission, and more.

GridTools gave users the added benefit of being able to easily run predefined tests upon a set of resources. GridTools could do such things like query Globus Toolkit gatekeepers or information services or perform GSI-ftp transfer tests, and then aggregate all this information into a common view that showed which parts of our testbed infrastructure were not performing as expected. Since GridTools was created using a modular approach for test integration, with most of its core functionality stored in module libraries, it was very trivial to add new or manipulate pre-existing tests. Leading up to the HPC Challenge Awards at SC 2002 GridTools was extensively used to test, setup, and verify our large testbed infrastructure which included over 80 different production HPC resources and subsequently won the HPC Challenge Award for “Most Geographically Distributed Applications and Most Heterogeneous Set of Platforms.”

Mock et al. [8] describe a batch script generator that was used successfully from SDSC with Cactus, connecting to about 80 different machines for a demonstration performed at SC 2001. This script generator runs as a web application, not necessarily tied into portal, to generate all the batch scripts needed for the TeraGrid machines used during this demonstration.

Yoon et al. [9] describe the difficulties in launching applications on HPC systems. Their approach to solving this problem differs in two crucial aspects from the approach described here: First, it relies on web services instead of on tools that are already available on standard HPC systems which makes it difficult to quickly deploy their solution on a new HPC system. Second, the descriptions of the available resources (the machine database) are maintained in a distributed manner by the resource owners. This is highly problematic because these descriptions are often a low priority since the majority of users do not need them. As a consequence, errors in resource descriptions may not be corrected in a timely manner, rendering resources unusable.

This paper is structured as follows. In section II we introduce the Cactus Software Framework as model for the kind of applications that our infrastructure supports. In section III we introduce the Simulation Factory and describe its basic concepts, and elaborate on some implementation issues in section IV. We describe our future plans in section V.

¹Fungibility - A good or commodity capable of mutual substitution: <http://en.wikipedia.org/wiki/Fungibility>

II. APPLICATION EXAMPLE: CACTUS SOFTWARE FRAMEWORK

Cactus [1], [2] is a software framework for science applications which is used to simulate physical systems in many fields of science and engineering such as black holes and neutron stars in general relativity. As in other software frameworks, applications are built from separately developed and tested components. Cactus is an open-source, modular, and portable programming environment for collaborative high performance computing (HPC). It was designed and written specifically to enable scientists and engineers to develop and perform the large-scale simulations needed for modern scientific discovery across a broad range of disciplines.

The Cactus code base is structured as a central part, called the *flesh* that provides core routines, and components, called *thorns*. The flesh is independent of all thorns and provides the main program, which parses the parameters and activates the appropriate thorns, passing control to thorns as required. By itself, the flesh does not do any science; to do any computational task the user must compile in thorns and activate them at runtime.

A thorn is the basic working component within Cactus. All user-supplied code goes into thorns, which are, by and large, independent of each other. Thorns communicate with each other via calls to the flesh API or, more rarely, custom APIs of other thorns. The Cactus component model is based upon tightly coupled subroutines working successively on the same data, although recent changes have broadened this to allow some element of spatial workflow. The connection from a thorn to the flesh or to other thorns is specified in configuration files that are parsed at compile time and used to generate glue code that encapsulates the external appearance of a thorn. At runtime, the executable reads a parameter file that details which thorns are to be active and specifies values for the control parameters for these thorns.

The current version of Cactus provides many computational modules for finite difference based methods and has been very successful as indicated by the large number of scientific publications it has enabled. There exist currently (July 2010) more than 500 thorns in over 50 arrangements at various sites worldwide, many of which are publicly available. An international consortium has recently (June 2010) released the Einstein Toolkit [10], a complete, production-level, open-source set of components for relativistic astrophysics simulations that uses Cactus framework. We describe some details of the component structure of the Einstein Toolkit in [11].

Most researchers who use Cactus are developing their own code, combining both public and self-written components. This mode of work, whereas an existing code base is easily augmented by new modules, is made possible by Cactus's component structure which does not require nor permit any kind of centralized control. Researchers working in this way then need to build and run their code on various platforms. We depict the resulting life cycle of a simulation science project in figure 1.

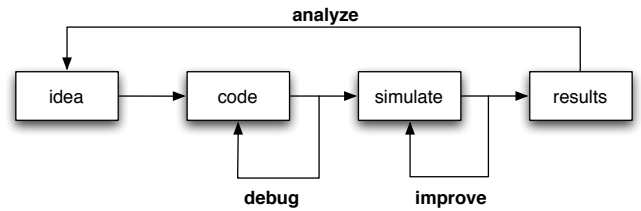


Fig. 1. General life cycle of a simulation, beginning with an idea, proceeding to a code development stage and then a production simulation stage, and ending with simulation results being post-processed and analyzed.

As an interesting side note, we want to remark that we have a sizable number of computer science researchers who are using Cactus. These researchers are often not familiar with the day-to-day usage of HPC systems since they have never been trained in the corresponding low-level details, and thus cannot undertake research in real-world systems. Nevertheless, these researchers are important for developing new capabilities with a sound theoretical backing. It is often difficult, if not impossible, to close the gap between a prototype and a real-world implementation.

Using HPC systems to perform simulations is similarly a complex task. These systems are run in *batch mode*, where one has to prepare a shell script that runs the actual code, and then submit this script to a batch system. After some time (hours or days), the script is executed, and its output and error messages are returned to the user. It goes without saying that debugging such scripts is very time consuming due to the long turn-around time and any user error can delay a simulation project by several days.

To add insult to injury, the maximum possible run times in such queuing systems are usually measured in hours, and not more than two days at best. This needs to be compared to production-level simulations that can require run times of the order of weeks. To deal with this, a simulation has to *checkpoint* itself before its queue time runs out and then *restart* when it receives another time slot in the batch system. In addition, if one uses a large number of nodes, there is an increased chance of system failures that will also require checkpointing and restarting. Automating the corresponding frequent re-submissions to the queuing systems is called *job chaining* or *presubmission*. Dealing with queuing systems can be very stressful for human beings because even small errors can invalidate or destroy weeks of simulation results. Each simulation day may consume 10k to 100k of CPU hours, corresponding to \$1k to \$10k in US currency (if bought on the free market).

The problems described here exist on all commonly available HPC systems and exist for virtually all current HPC applications (including Cactus). It is clear that this situation is highly unsatisfactory and that there is a dire need to shield the user from system-level details and low-level simulation maintenance operations.

Once a researcher has moved from postdoc to faculty, he or she usually does not have the time any more to use HPC systems daily. Once this practice is gone, it is very difficult

to get “back into the groove”, leading to highly unsatisfactory situations where faculty (who often originally developed the software!) cannot use them any more.

III. SIMULATION FACTORY: BASIC CONCEPTS

SimFactory evolved as an application to manage the idiosyncrasies present in HPC systems. The complexity found herein is a result of the uniqueness of each of these machines and in the uniqueness of the codes users deploy there. Real-world input from these users allowed SimFactory to move beyond a prototype and into a practical, pragmatic application that truly aids non-computer-science research. While the design of SimFactory may seem overly complex in places, this only reflects the complexity that exists in the world of high performance computing.

SimFactory addresses three main goals: *source code management, configuring and building simulations, and managing and executing simulations*. Building on a Machine Database, SimFactory can accomplish these goals consistently and transparently across any pre-configured HPC resource. Each of the three main goals contains unique challenges that we describe below. Figure 3 below describes the lifecycle of a simulation as it directly relates to simfactory commands.

A. Managing Source Code

Many research codes are developed in an open and/or collaborative manner, where end users not only use applications, but also make modifications or add their own modules. This is in particular facilitated by the component model of the Cactus framework (see section II above) that we use as model application here. A user may start with a certain version of an application code, make these modification on a workstation or notebook, and then move on to an HPC resource after some testing.

While doing so, it is important to keep track of the different versions and modifications of the application source tree. It is usually not possible to use version control systems at this stage, because (a) the user may lack direct write permissions to the repository, or (b) the repository rules accept only well-tested and finished changes. To facilitate development that spans multiple machines and testing on different platforms, SimFactory offers the following model:

- the user chooses a single *home system* where he/she performs all code development;
- this home system contains the *authoritative version* of the source code, or contains multiple versions in different directories;
- all other systems are set up as *mirrors* of the home system, i.e. usually the source trees on these systems is not directly edited;
- SimFactory provides a convenient (easy and quick) method to *synchronize* (mirror) source trees.

In particular, this implies that one accesses code repositories (cvs, svn, git, ...) only from the home system. The code base can consist of components that are hosted in many different

repositories. SimFactory will then replicate this source tree structure from the home system to remote systems.

Compared to a more “traditional” development model, where one checks out the source code on multiple systems, this has several advantages. First, all authoritative source code versions are located on a single system where they can be easily compared, backed up, etc. Second, source trees on different systems cannot diverge accidentally since SimFactory’s mirroring command can keep them up to date. In addition, our build environment (see section III-B below) automatically tags and captures source trees as executables are built, so that one can recreate the source tree that was used to build a certain executable.

Duplicating a source tree to a remote system requires knowledge about remote access methods, authentication, directory names, etc.; SimFactory accomplishes this goal by facilitating remote access and authentication with the remote resource using a pre-configured authentication mechanism such as *ssh* or the *Globus Toolkit*. If the remote system is not world-accessible, SimFactory uses “trampolines” (one or more intermediate, authorized machines) to complete a trusted authentication chain. Building on these mechanisms, SimFactory performs the actual synchronization using *rsync* or a comparable mechanism. It should be noted that this mechanism requires typically only a few minutes with a cold file cache, and under ten seconds with a hot file cache.² We show example timing results in figure 2.

This synchronization replicates not only source code but can also replicate parameter files and input files

B. Configuring and Building

Before running simulation one has to configure and build an executable from the source tree. These steps typically cannot be performed automatically and require user input; often, a complex set of inter-dependent configuration variables has to be set. In fact, this step is often so complex that only experts are able to configure and build an application on a particular system even if the applications themselves are portable.

There are two kinds of configuration settings for an application. Some configuration settings select features of the application (e.g. whether a certain component is to be included, or what level of optimization should be used). Other configuration settings are determined by the host system and have to be chosen “just right” to make everything work (e.g. compiler version, compiler flags, paths to external libraries, etc.)

Tools that are commonly used to help configuring and building applications are either not available on or not applicable to HPC systems. System-level tools such as *rpm* [12] or *apt* [13] are not provided on HPC systems, and cannot be installed by end-users. User-level tools such as *autoconf* [14]

²This assumes that there are only few modifications to the source tree, as is usual during a edit-compile-test cycle. These times depend greatly on the file system. A cold cache refers to the first time these files are accessed in the edit-compile-test cycle, which requires the files be read from disk, and a hot cache refers to the files being in memory in the file system cache.

Machine	Location	full/cold	full/hot	update/cold	update/hot
numrel10	CCT (local)	52	40	5	5
Eric	LONI	57	40	5	4
Queen Bee	LONI	64	64	7	7
Kraken	NICS	2277	1955	14	15
Ranger	TACC	112	106	23	16

Fig. 2. Source-tree synchronization timings. (All times in seconds, rounded to the nearest second.) This measures synchronizing the complete Einstein Toolkit [10] source tree from a machine at the CCT (LSU) to the specified machine. This source tree consists of about 50k files with about 450 MByte. (“full” copies the tree for the first time, “update” has the source tree already present on the destination; “cold” and “hot” describe the state file system cache.) In all cases, updating an existing source tree takes only a few seconds. The initial copy on Kraken takes an inordinate amount of time; this is a property of Kraken’s file system and is also seen independent of the Simulation Factory.

do not work well because (a) existing software is often installed in non-standard locations, (b) several fundamentally different versions of a particular package may be available, requiring a user choice (e.g. between Intel and PGI compilers), and (c) testing whether a feature is present or not may require executing an application which may require using a batch system to submit a job with a turn-around times measure in hours. (Thus `autoconf` may require days to complete.) Finally, `autoconf`’s approach of simply trying out whether a feature is available may be considered abuse of the system and be disallowed by usage policies.

CMake [15] has features similar to `autoconf`; there is no provision for a database that would store machine-specific configuration details.

Most HPC systems allow user-level configuration tools such as SoftEnv [16] or Environment Modules [17]. These packages allow users to choose between several installed software versions (e.g. different compilers), and (if set up properly) will ensure that all enabled software packages are compatible with each other. Unfortunately, SoftEnv settings are global to a user’s account, so if a user builds an executable, and then switches his/her SoftEnv settings while this executable is waiting in a queue, the job may crash when it finally starts since important libraries may not be available any more. Environment Modules remedy this flaw but they still do not provide sufficient information to (a) choose a particular version of a module, or (b) select good compiler options for this version. It is also not possible to automatically determine what library a particular module provides, as only a module’s name is available – the BLAS [18] library may e.g. be provided by modules called `acml` [19], `atlas` [20], `essl` [21], `gotoblas` [22], or `mk1` [23], (and none of which provide the Netlib reference implementation [18]). Similar ambiguities exist with choosing a compiler or with choosing an elliptic solver if the application supports several interfaces (e.g. both PETSc and Hypre). And in the end, there may still be incompatibilities due to errors or mis-interpretations between any of these or any of these and the application, which may only be detectable as crashes at run time.

What this all amounts to is that one has to carefully study a system’s documentation and perform careful experiments to find good, working configuration options.

SimFactory stores the complete configuration information for every machine (for a given application) in its machine

database. This allows everybody (including new users) to quickly build the application on every supported system. This configuration information is thus, in its entirety, “blessed” by its corresponding maintainer, providing a service to the community. This approach is in contrast to a design where the simulation factory would pick up bits and pieces of configuration information automatically from the host system and would then combine the configuration information by itself; this approach lacks the “seal of approval” that exists in the current approach. Given the complexity of identifying a correct set of configuration information for a particular system, where even small details can uncover compiler errors or lead to inconsistencies between different libraries, such a seal of approval is crucially important.

The disadvantage is that this approach does not scale well – it requires one maintainer per application per supported system and the Cactus configuration information with about 30 supported production system is reaching this limit. We suggest to address this in two ways: In the short term, we assume that each user community will maintain their own machine databases, limiting the number of systems that need to be supported in each of these. In the long term, we expect resource providers to maintain more and more details about their systems in formal descriptions in a reliable manner, so that parts of the machine database can be determined automatically.

The Cactus framework supports building multiple executables from the same source trees. Each of these executables is called a *configuration*, since they differ in the configuration settings that were used to create them. These configuration settings include a *thorn list* (list of components that should be included into the configuration), and a set of high-level build options such as *debug*, *optimise*, or *profile*. These configurations have different names, allowing the user to specify which configuration to use when performing a simulation.

In many cases, a single SimFactory command suffices to create a Cactus executable from a given thorn list and the very same command works on any production machine that a research group may be using. This is a substantial simplification over the previous state of affairs and allows every Cactus user to add or modify code and then re-build the configuration with only minimal effort.

C. Managing Simulations

Once a configuration has been created, SimFactory provides functionality for performing simulations, either by submitting and managing jobs via a job queueing system, or by directly running the executable.

The simulation factory follows a high-level abstraction for performing simulations. In this abstraction, performing a simulation consists of many more operations than just running the executable. In particular:

- The first step is to *create a simulation*, which captures an executable, a parameter file, any input files there may be, as well as any other parameters that determine the physical result of the simulation. This excludes any incidental parameters (see below), and does not actually start the simulation.
- To make progress with the simulation, one either submits or runs a *restart* (roughly equivalent to a “job” in a queueing system). This requires choosing incidental parameters, such as the number of processes, wall time limit, allocation/queue names, etc. At most one restart can be active at one time.
- After the restart finishes, it is *cleaned up*, which may consist of minor actions such as correcting file permissions, or deleting unnecessary or broken files, or may e.g. automatically archive simulation results.
- A simulation may consist of arbitrarily many restarts. Presumably, each restart continues where the previous restart left off. (This is necessary since queue time limits on HPC systems are often much too short to complete a simulation.)

Figure 3 shows the life cycle of a simulation and its restarts graphically.

This high-level model for performing a simulation differs in certain crucial respects from a “naive” way of doing so. First, it distinguishes clearly between those parameters that influence the scientific result and those that are only incidental. Second, the simulation factory explicitly captures all parameters and necessary input (by copying) so that one cannot accidentally modify these parameters while a simulation is running, which can be a time scale of many weeks. Third, it introduces the notion of a clean-up step after each restart has run, providing a hook for additional actions, such as automatically archiving results.

Finally, the simulation factory performs these details automatically, consulting the machine database to be able to map these details onto a particular system. By performing these actions automatically, (a) each simulation (within a research group) is performed in a consistent manner, allowing others to understand the directory layout and access the results, (b) users are relieved of performing many tedious low-level tasks manually, and (c) many errors and accidental omissions are avoided. By implementing best practices in the simulation factory, the often unwritten experience of users is captured, resulting in simulations that are “naturally” performed in the “best possible” manner, including e.g. capturing all necessary

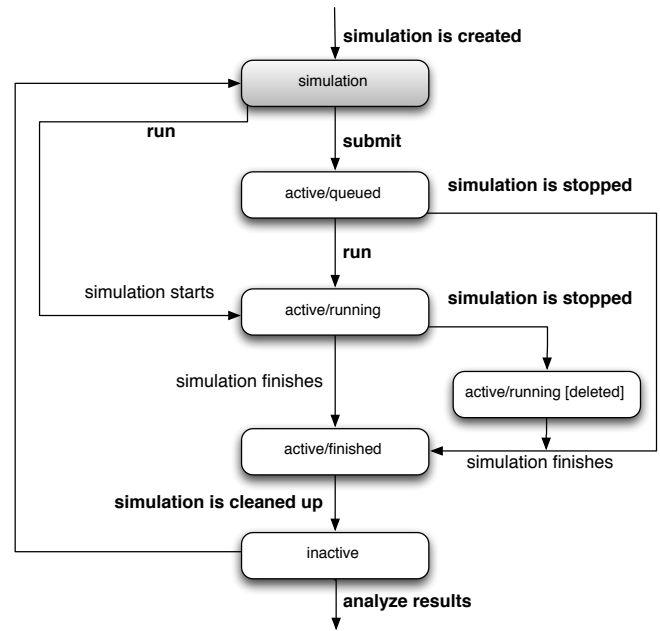


Fig. 3. Simulation Workflow. This shows the life cycle of a simulation, starting from its creating, proceeding potentially through several restarts, until it is finished. The bold text directly corresponds to SimFactory commands.

provenance information to make simulations truly repeatable.

In detail, the simulation factory performs the following actions:

- create and populate a directory structure for the simulation;
- copy all executables, parameter files, and input files to save them from accidental modification (ensuring to avoid superfluous copies to save disk space);
- manage checkpoint files, and/or ensure the correct checkpoint files are used when restarting;
- allow *presubmitting* (or *chaining*) of restarts, i.e. submitting several restarts at once that will then automatically be executed sequentially (if and as allowed by the queueing system and system policies);
- allow to run executables directly or interactively, potentially using “interactive queued jobs”;
- use and/or create unique identifiers for simulations and restarts, so that output files can be tagged pointing back to the exact simulation;
- automatically archive simulations and restarts, since files on HPC systems are often automatically deleted after some time;
- clean up in various minor but convenient ways, e.g. correct file permissions or delete unnecessary output files.

D. Information and Status Inquiries; Provenance

In addition to the actions supporting source tree management, configuring/building, and managing simulations, SimFactory offers commands to display information and inquire about the status of simulations and restarts. This includes displaying Machine Database entries and configuration infor-

mation. This allows the user to monitor simulations, know when they are completed, and check and restart them if they are interrupted. This also provides access to the list of the HPC resources that have been pre-configured, allowing the user to know which HPC resources they can begin using immediately.

In performing the actions described above, SimFactory keeps a log trail associated with each simulation, describing all steps that led to a particular simulation state and the order in which they were taken. SimFactory also keeps safe copies of all executables and input files that were used for a particular simulation so that changes to these files outside of SimFactory’s control do neither affect currently ongoing simulations nor confuse the log trail.

Furthermore, SimFactory generates and manages unique identifiers for each simulation and restart and passes these and other provenance information on to the application which can then e.g. tag output files and images. SimFactory also understands provenance information generated by the application, which is stored together with application output and which is displayed to the user together with other application output.

E. Machine Database

The main idea behind SimFactory is to provide a resource agnostic tool that is able to take full advantage of the various HPC resources available to researchers. To separate SimFactory from the resource on which it is used, we employ a *machine database*, which is a collaborative database compiled by SimFactory maintainers, researchers, and other users that stores all machine dependent information. This database is of crucial importance to SimFactory’s design (see section III-B above).

Each machine database entry is broken out into four groups:

- *Machine description*: information about the machine itself, used for logging/informational purposes;
- *Machine access*: parameters defining remote access and management of the resource, e.g. defining how to log in or to synchronise files and directories;
- *Source tree management*: parameters for defining a good directory for the source tree, the default make command, and what the default configuration options are;
- *Simulation management*: parameters containing information on how to submit, manage, and run simulations using the resource’s specific job queueing system.

This database provides the user the ability to run SimFactory on any known resource. We use the word “known” because the Machine Database is a collection of pre-defined settings that represent the knowledge SimFactory must have in order to configure, build, and run simulations. The Machine Database provides the ability to deploy simulations quickly and efficiently.

IV. IMPLEMENTATION ISSUES

Below we discuss some interesting challenges that had to be addressed in the design and implementation of SimFactory. Specifically, we will focus on the evolution of SimFactory to its current state, the method used by SimFactory to become

machine agnostic, the abstraction we use to communicate SimFactory’s command line options between its modules, the restart abstraction, which represents how SimFactory encapsulates a specific stage of a simulation and finally how SimFactory represents presubmitted jobs internally, which involves creating and submitting multiple jobs to a job queuing system to handle simulation wall times greater than the maximum allowed wall time for a single job.

A. History

SimFactory was originally designed for SC 2006 to simplify executing sets of benchmarks on many HPC systems, and was implemented as a monolithic Perl script centered around the Machine Database. The Machine Database was implemented as Perl hash table initialized via executable Perl code. The three different tasks (source code management, configuring and building, simulation management) existed from fairly early on, as did the distinction between a simulation and a restart. Advanced features such as presubmission was “tacked on” later and didn’t quite fit the original abstract model of a simulation, and neither did running a restart without submitting it to a queue. In addition, after growing a user base, maintaining the Machine Database and its necessary local modifications in executable Perl code was not attractive any more.

While updating the abstract model of a simulation, we decided to restructure SimFactory’s internal implementation and to switch to Python as implementation language because several of the main users and contributors requested so.³ One of the main features of the SimFactory is that it can run everywhere without being installed (just downloading or copying must suffice), which essentially leaves only Bash, Perl, or Python as implementation languages. We found that most HPC systems run Python 2.3 or later – this also nicely demonstrates the extremely conservative time scale on which HPC systems install or update software.⁴

We rewrote SimFactory in Python as an object-oriented, module-based application. SimFactory consists of four separate modules, corresponding to the features described in the subsections of section III above. Each module can either be called directly by the user, or can be dispatched as an imported module by a (future) GUI application. SimFactory currently includes one command line UI application called `sim`, maintaining command-line compatibility with the previous version while also providing access to new functionality. Each of these four main modules relies heavily on the Machine Database to provide information about the HPC resource on which it is executing.

³The main reasons cited for preferring Python was the cleaner syntax and the more elegant modern facilities to support large-scale programming, such as classes and modules. One reason cited against Python was that it does not perform a static type checking at startup, so that uninitialized variables are only detected at run time.

⁴Python 2.3 was released in 2003; we write this paper in 2010.

```
# a block of text

# Official Cactus entries
sync-sources    = <<EOT
CONTRIBUTORS
COPYRIGHT
Makefile
arrangements
src
lib
EOT
```

Fig. 4. Example of a multi-line block of text in the machine database, listing multiple directory names for the key `sync-sources`.

B. Machine Database Details

1) *File Format*: As described in section III-E above, the machine database describes properties of each machine so that SimFactory can provide a resource-agnostic user interface.

The HPC user community dislikes non-human-readable file formats for non-performance critical information. We therefore use the INI file format [24], extended to support multi-line block text entries similar to “here” documents found in Bash and Perl. Figure 5 shows a partial entry for a particular machine, and figure 4 demonstrates a multi-line entry. Multi-line block entries use `<<` followed by any sequence of characters and then a newline to indicate the start of a block. To end the block, the same sequence of characters following `<<` must be repeated on a line by themselves.

We chose this file format because it is both readable and portable. The INI file format is platform agnostic, clear-text, and easily understood, created, and edited because of its simple syntax.

2) *Implementation*: The Machine Database is comprised of a set of entries with predefined keys, separated into sections with unique names for each machine, as shown in figure 5.

We anticipate that users will have to maintain local modifications of the Machine Database, typically to define their user names and allocations on these system. To facilitate this, SimFactory provides the user with the ability define global defaults in a `[default]` section, as shown in figure 8. Settings defined here propagate to all Machine Database entries. Users can also provide new Machine Database entries, describing e.g. private systems such as personal workstations or notebooks, and can overwrite specific keys in the Machine Database. Figure 7 demonstrates how to define a different user name and thorn list, which will also override the value in the `[default]` section, for a pre-defined Machine Database entry.

The Machine Database comes pre-configured and is maintained by the developers and maintainers of SimFactory. The last database, the User Database, is where the user makes their edits, adds their local workstation if necessary, and defines necessary default values that will propagate throughout each of the three databases.

The databases are located in the SimFactory source tree

```
[queenbee]

# Machine description
nickname       = queenbee
name           = Queen Bee
location       = LONI, LSU
description    = The large LONI Linux clu...
webpage       = http://www.loni.org/...
status        = production

# Access to this machine
user           = YOUR_LOGIN
email         = YOUR@EMAIL.ADDRESS
hostname      = qb4.loni.org
rsynccmd      = /home/eschnett/rsync-3.0...
sshcmd        = ssh
localsshsetup = :
sshsetup      = :
aliaspattern  = ^qb[0-9](\..loni\.org)?$

# Source tree management
sourcebasedir = /home/@USER@
...
```

Fig. 5. Example partial Machine Database entry in the human-readable INI file format. This is taken from the entry describing Queen Bee, a shared LONI/TeraGrid system in Baton Rouge, LA.

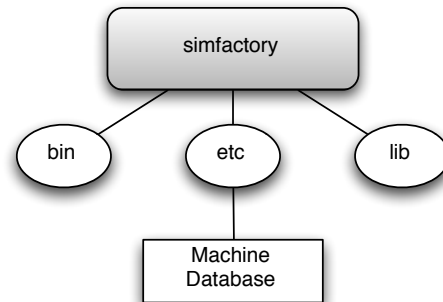


Fig. 6. Simulation Factory db file structure.

```
# override some mdb entries
[queenbee]
user           = mthomas
thornlist      = einstein-bassi.th

[is]
user           = mthomas
thornlist      = einstein-numrel-intel.th
```

Fig. 7. Machine database syntax: Specifying a different user name for certain machines in the machine database.


```
# Defaults for all machines
[default]
user      = mwt
email     = mthomas@cct.lsu.edu
allocation = loni_cactus04
```

Fig. 8. Machine database syntax: Defining default values to override entries in the machine database.

inside the `etc` folder, as seen in Figure 6.

C. Macros

Machine database entries, option lists, script files, and other files that are processed by the SimFactory can contain macros that are replaced at run time. For example, every instance of `@USER@` found in the `[queenbee]` Machine Database entry (see figure 5) will be replaced by the username `mthomas`, as specified in figure 7. This allows the user the flexibility to set the user name once and use it in a generic manner for any other user-name dependent parameters needed by SimFactory.

In addition to a set of predefined macros that correspond to Machine Database entries or values gathered from the system (such as e.g. a simulation job id), one can also define additional, arbitrary macros via command line options to SimFactory.

D. Restarts

One unique challenge SimFactory addresses is how to manage multiple stages of a single simulation, whether the stage represents a fresh start or a recovery from a previously interrupted simulation. To address this, SimFactory contains an abstraction called *restart*. Figure 3 in section III-C above shows the typical life of a SimFactory restart. A restart encapsulates several key operations:

- *create*: Before a simulation can be submitted or executed, it must be created. This process initializes any required configuration parameters, directories, and any other infrastructure necessary to facilitate submission or execution.
- *submit*: The submit operation submits the simulation to the queueing system of the host system. A shell script file is the command that is sent for submission. This script contains the necessary options to initialize the queueing system correctly, such as choosing the correct wall time, and then commands calling the SimFactory `run` operation. This submit operation does not contain any execution logic.
- *run*: The run operation is where all execution logic lives. The run command is capable of launching simulations that have either been submitted in a queuing system, or are executed directly, without the use of a queueing system. The ability to execute a simulation directly is necessary for running small simulations on a local workstation or notebook. The run operation uses the `mpirun`

command specified in the Machine Database. This command can be any shell command, such as the actual `mpirun` command to launch a job using the system’s MPI implementation, or just the simulation binary itself, skipping the use of the MPI altogether.

E. Presubmission

One of the most important challenges SimFactory has to address is the need to execute simulations automatically beyond the maximum execution time allowed on the HPC resource. To facilitate this, SimFactory determines, based upon the specified and maximum allowed wall time, how many submissions to the queueing system are necessary. SimFactory then submits the job this many times and then sets up the necessary daisy-chain to make the simulations launch in the correct order. A simulation checkpointing system, which allows a simulation to resume where it has left off, is necessary for presubmission.

V. FUTURE PLANS

We plan to extend the feature set provided by SimFactory to include managing simulation output, i.e. often large output files that are “left behind” after simulations have finished. Managing simulation output also depends on low-level machine characteristics, such as after how much time it will be deleted automatically, what commands have to be used to access it efficiently, and what long-term storage mechanisms can be reached from the simulation machine. Other challenges include ensuring that simulation output files and post-processing results remain “together”, so that one can reliably trace back to the root of the simulation e.g. from a figure found in a publication or an image found on a web site. This topic involves repeatability of numerical calculations and provenance of numerical data, and the SimFactory is an ideal vehicle to implement the corresponding low-level mechanism to spare the user these details.

Another possible extension of SimFactory is to support simulations running across multiple sites or off-loading certain ancillary (analysis) tasks to secondary machines to reduce the load on the primary machine. In the past, several of the issues relating to identifying such tasks in the Cactus framework were addressed [25], [26], but reliably being able to mirror the source code onto remote systems and reliably starting new simulations there remained an unsolved problem. This will be an ideal application case for the SimFactory.

While SimFactory is currently targeting the Cactus framework, it is clear that the issues it addresses and the solution it offers are relevant for many other applications as well. We intend to abstract out all application-specific bits into an *application database* so that SimFactory can support other applications as well, as long as these require any of the same basic features (access to remote systems, source code management, simulations on HPC systems).

Other simulation packages (e.g. Enzo, ADCIRC, NAMD, etc.) face very similar issues. If a package is used only as “black box” on an HPC system, without making modifications to its source code, one can use a pre-installed copy of the

executable which often mitigates these problems. However, it is the nature of graduate student research that new methods and new algorithms be tried out and these will then have to face the issues. The basic workflow (build and test on local system, build and test on HPC system, submit and manage a set of jobs, handle checkpointing and restarts) is virtually identical for most simulation packages. We have recently begun to investigate SimFactory support for ADCIRC [27] [28], which is used to model storm surges caused e.g. by hurricanes in the Gulf of Mexico.

While the SimFactory provides the infrastructure (middleware) for the features it offers, it also provides only command-line interfaces. Graphical User Interfaces (GUIs) would provide several obvious advantages; first, guiding the user to possible next steps for each state (making SimFactory easier to use for beginners), and second, providing visual feedback about the current state and keeping it updated automatically, without requiring a user command and the lag time thereafter. The (command line) user interface logic is separate from the application logic, which will allow us or others to offer a GUI, based e.g. on QT [29] or GTK [30], or via a web service. We are also currently implementing a TeraGrid Gateway [31] for numerical relativity that will use the Simulation Factory.

Since being accepted, this work has also been presented as a poster at TeraGrid '10 [32].

SimFactory is released under an open source license and is freely available as part of the Einstein Toolkit, as described on <http://einstein toolkit.org>.

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