Near Real-time Data Analysis of Core-Collapse Supernova Simulations With Bellerophon

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Abstract
We present an overview of a software system, Bellerophon, built to support a production-level HPC application called CHIMERA, which simulates core-collapse supernova events at the petascale. Developed over the last four years, Bellerophon enables CHIMERA’s geographically dispersed team of collaborators to perform data analysis in near real-time. Its n-tier architecture provides an encapsulated, end-to-end software solution that enables the CHIMERA team to quickly and easily access highly customizable animated and static views of results from anywhere in the world via a web-deliverable, cross-platform desktop application. In addition, Bellerophon addresses software engineering tasks for the CHIMERA team by providing an automated mechanism for performing regression testing on a variety of supercomputing platforms. Elements of the team’s workflow management needs are met with software tools that dynamically generate code repository statistics, access important online resources, and monitor the current status of several supercomputing resources.

Keywords: data analysis, visualization, core-collapse supernovae, n-tier architecture, software engineering, usability, workflow management, artifact management

1 Introduction

Leadership-class simulation science is already, at the petascale, an enterprise fraught not primarily with concerns regarding raw computational power, but rather, with problems concerning the generated data and the human interactions required to obtain scientific insight from these data. The sheer volume of data, policies designed to ensure their integrity, and efficient methods to interpret them are immediate obstacles faced by almost all computational scientists running capability-class simulations.
Most importantly, little of this bleeding-edge computational science is done by individuals alone, or even within very small teams in close physical proximity. In addition, these teams are often augmented by individual researchers who need access to the simulation data to further the scientific aims of the project. This access is often hampered by (necessary) security policies at the computing facilities, and, more often than not, requires third-party intervention (i.e., a consultant must be called on the phone and UNIX permissions are set by hand for a period of time). All of these difficulties often occur in an environment of rapid and incessant code development. The nature of computing at leadership-class facilities invariably leads to teams of developers and users working in concert. Indeed, these groups rarely have sharp divisions, i.e., users of the codes are often the primary developers as well. Intensive code development, constant (with a cadence of less than 18 months over the last decade) platform evolution, growing data volumes, and higher and more serious data security concerns have all led to a situation in which computing on the world's largest supercomputers is a daunting task for the most sophisticated computational scientists.

Over the past decade, research efforts anchored at Oak Ridge National Laboratory (ORNL) have resulted in the development and deployment of several codes designed to perform simulations of core-collapse supernovae. The current production “workhorse” for the group is the CHIMERA code [1]. CHIMERA is used in production mode on a variety of supercomputer platforms to perform two- and three-dimensional simulations. The code is typically run with as few as 256 Message Passing Interface (MPI) tasks to as many as 131,000 tasks, and at a variety of sizes in between, depending on the dimensionality of the simulation and the resolution used in space, neutrino phase space, and nuclear network size. Typical simulations can produce between 30 Gigabytes (GB) to well over 80 Terabytes (TB) of data per run. In these ways and others, CHIMERA is a typical leadership-class simulation code. Importantly, the nature of the CHIMERA collaboration itself - a moderately sized development team with a large overlap between developers and users - is also common among other HPC application efforts. In addition to the developers located at ORNL, major outposts of development exist throughout the United States. These developers have produced an application that has well over 250,000 lines of code. Consistent, efficient production at leadership scales requires near-constant code development, and any code changes must be motivated by scientific targets. Unfortunately, with only a few geographically dispersed investigators to accomplish both tasks, the wrangling of TB's of data to gain scientific insight and the incessant need to manage enterprise-scale code development has already proven to be impossible without the help of a sophisticated software system designed to facilitate both tasks at once.

Bellerophon is a support system developed at ORNL over roughly the past four years to address precisely these challenges with a goal of automating data analysis, workflow management, and software engineering tasks. It has enabled the CHIMERA team to discover and isolate multiple bugs and other subtle issues. It has also resulted in a direct impact on simulation results and facilitated several publications [2, 3]. Bellerophon is an integrated system of standalone, reusable subcomponents, tools, libraries, and services deployed across several supercomputing facilities, a dedicated web and data server, and multiple client-side implementations, providing an encapsulated, end-to-end software solution. The design of Bellerophon’s n-tier architecture includes a logic, data, and presentation tier as well as a supercomputing tier as seen in Figure 1. Elements of the supercomputing tier monitor simulation progress, process and analyze results, archive data, and transmit new data to Bellerophon’s data server in near real-time. Components from Bellerophon’s supercomputing tier have been ported and installed on Titan at the Oak Ridge Leadership Computing Facility (OLCF), Kraken and Darter at the National Institute for Computational Sciences (NICS), and Hopper and Edison at the National Energy Research Scientific Computing Center (NERSC). These installations also integrate the High Performance Storage System (HPSS) associated with each supercomputing platform. Bellerophon’s logic tier and data tier components, which reside on a dedicated web and data server, are responsible for processing data received from the supercomputing tier and enabling authenticated access to source data and analysis artifacts via a secure PHP web
service. The client-side implementations, which form the presentation tier, include a web-deliverable Java desktop application and, currently in development, Android phone and tablet apps.

Other data analysis and workflow management systems with user-friendly clients have been developed for HPC applications. For example, the Electronic Simulation Monitoring System (eSiMon) [4, 5] is a web-based dashboard system enabling a collaborative environment for scientists to monitor simulations and analyze their results. Users of eSiMon can determine system and job status, list and archive simulation runs, manipulate data, and automatically generate customized renderings of this data changing over time. Built using the Adobe Flex framework, eSiMon is a cross-platform Flash application designed with a user-centric theme. Kepler is another workflow management software system that provides users the ability to design and execute scientific models and automatically analyze and share output data [6, 7]. Kepler’s cross-platform, Java-based client application offers highly interactive tools to graphically create reusable, nested workflows integrated with essential software components. Kepler natively supports parallel processing and interfaces with several grid technologies including Globus, SRB, Web, and Soaplab Services. Another Java-based system, the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program’s Integrated Computational Environment (NiCE) [8, 9] provides tools to interactively analyze and visualize input and output data from a variety of nuclear reactor simulation types using rendering engines such as VisIt [10] and swt-xy-graph [11]. NiCE also provides Java and C++ APIs for reading and writing this data to the HDF5 format [12]. All of these workflow systems share characteristics with Bellerophon, but none offer the ease of use and specific developer-user hybrid features we have built into Bellerophon. Our design aim has been to provide a CHIMERA development and simulation tool first and foremost, with a plan to extend Bellerophon for general use in the future. This stands in contrast to the general nature of tools like eSiMon and Kepler, each of which was designed for use by multiple codes and teams from the outset.
2 Near Real-time Data Analysis

Bellerophon’s automated data analysis capability provides robust access and customization of animations and plots generated concurrent to ongoing CHIMERA simulations. Encompassing all tiers of Bellerophon’s architecture, this system seamlessly binds results from ongoing simulations, or archived results from previous runs, with the logic, data, and presentation tiers. A wealth of provenance metadata stored with the animations uniquely links them to the simulation model and contains information regarding the platform, job, data location, and time of creation for each frame produced. Creating and customizing visualization artifacts is simplified with the Visualization Set Manager tool accessible from Bellerophon’s client-side Java application. Another tool, the Visualization Set Explorer, provides users the capability to load and play animations in a viewer with VCR-like controls, to create custom frames dynamically, to download QuickTime-compatible MP4 movies (including frames as Portable Network Graphics (PNG) images), and to access provenance metadata for each frame.

2.1 Supercomputing Tier Subsystem

Bellerophon’s near real-time data analysis and visualization capabilities provide the CHIMERA team direct insight into the production runs. Once a run is bound to Bellerophon, a simulation’s results are processed, rendered, and viewed with a latency as low as five minutes through the client-side application. A central component of the supercomputing tier subsystem is the data_generator program, which is launched as a serial process from within the PBS script for a CHIMERA job (see Figure 2). Once a single configuration file is customized, this program monitors the simulation for new data, executes data analysis or conversion programs when new data is detected, and transmits the modified results and other metadata to the remote data server. This metadata includes the name of the supercomputing platform, the full paths to the run’s input and output data files, and the job’s start time. Once the data_generator has accessed information from Bellerophon’s remote server, it begins monitoring CHIMERA for new data to process. The data_generator currently utilizes two executables, chimera2silo and Chimeralyzer, to process simulation results. The chimera2silo program converts selected CHIMERA binary output to the Silo data format [13]. Chimeralyzer performs time-sequenced analysis of CHIMERA output and exports important tabulated quantities such as shock radius, gain radius, and proto-neutron star (PNS) radius vs. time, three measures of explosion energy vs. time and temperature vs. radius over time. Analyzing these quantities is essential to CHIMERA development.

Figure 2: A flowchart detailing processes within Bellerophon’s supercomputing tier.
because explosion energy is the primary indicator of the efficacy of the explosion mechanism and the shock, gain, and PNS radii outline the supernova heating profile. The data_generator transmits the Silo files and data sets to the data server and archives a copy of the results in the supercomputing platform’s mirrored storage area for Bellerophon’s data. Another program, data_archiver, creates a compressed copy of this storage area and transfers it to the platform’s HPSS using the HTAR utility on a weekly basis. Since CHIMERA is a long-running simulation that rewinds before each restart point, the data_generator program is also responsible for keeping Bellerophon’s archived data for each run up to date. If the program automatically detects a restart point, it deletes all data within Bellerophon’s database past the associated restart cycle. Conversely, if new CHIMERA data exists that was not previously processed, the data_generator will automatically bring Bellerophon’s database up to date with the simulation’s current state.

2.2 Data and Logic Tier Components

In addition to the archives stored in systems within the supercomputing tier, Bellerophon’s data tier consists of a MySQL database and a flat file database comprised of a hierarchical set of directories containing processed CHIMERA output data and renderings of this data. An object model for this database, which links MySQL tables and records to Bellerophon’s data files, has been developed. The top-level object in Bellerophon’s data model is the visualization set. A visualization set is a collection of animations and visualization jobs with metadata tied to a unique scientific model. It also includes an associated data directory that contains the output files created by the data_generator program. An animation object represents how this data is rendered. It is comprised of customizable animation attributes, a rendering engine, and an associated media directory containing the resulting artifacts (e.g., PNG images and MP4 movies). A visualization job tracks the provenance of CHIMERA’s output data and renderings by processing metadata transmitted to the data server by the data_generator program for each batch job. This metadata includes the batch job’s id, supercomputing platform, input and output data paths, start and end frame numbers, and start and end wall times.

![Figure 3: A flowchart detailing elements and processes within Bellerophon’s logic and data tiers.](image)

Bellerophon’s logic tier is tasked with processing incoming data, rendering the data, and providing a mechanism to securely access the data and its artifacts through the Bellerophon web service (see Figure 3). Every hour, data and visualization processors on the server check for new post-processed output data and metadata files transmitted by the data_generator program. They process these files, update the relevant MySQL database tables, and render animations according to user-defined specifications stored in the database. Bellerophon’s logic tier components currently use two backend rendering engines: the VisIt Visualization Tool and Grace [14], a 2D plotting tool. VisIt is used to generate animated 2D colormaps of more than a dozen quantities over time. These quantities include temperature, density, pressure, entropy, and electron fraction. Bellerophon leverages Grace and the
ImageMagick library [15] to generate static 2D line plots of shock radius, gain radius, and PNS radius vs. time as well as three measures of explosion energy vs. time. It is also used to create animations of 2D line plots of temperature vs. radius over time. The Bellerophon web service allows authenticated users to access this database and execute other backend programs from a client-side application using a well-defined specification.

### 2.3 Client-side Analysis Software Tools

Bellerophon’s presentation tier is currently implemented as a cross-platform, digitally signed Java application, which is deployed over the network using Java WebStart technology [16]. Java WebStart enables installation and execution of the client-side user interface by simply clicking a hyperlink in a web page. Once launched, the application delivers a suite of easy-to-use software tools. Augmented by an aesthetically pleasing look and feel, its dashboard design employs the WYSIWYG (i.e., “What You See Is What You Get”) approach to graphical user interface development. Under this implementation of WYSIWYG design, users can access any function with only one or two mouse clicks. In addition, the user interface employs the windows wizard motif. In this design, users accomplish complex tasks in a simplified manner over multiple steps. Each step requires the user to enter a small amount of information or make one or more selections before going forward. Visual clues are also utilized in the Bellerophon Java client. Bellerophon’s intuitive use of icons, text, and color for each UI component enable users to quickly navigate to their desired selection. This emphasis on usability allows for remarkable ease-of-use, ease-of-adoption, and aesthetic quality.

In order to bind a particular CHIMERA model to the data analysis system, Bellerophon users must create a visualization set by entering some metadata describing the simulation and creating at least one figure.
animation using the Visualization Set Manager. Upon starting the manager, users have the choice of updating an existing visualization set or creating a new set. If the user decides to update an existing set then the visualization set selection user interface is displayed. This interface allows users to view all existing visualization sets in a table, filter the table by the sets’ attributes, and sort the table rows by these attributes. Once a visualization set is selected, the user can modify the set’s metadata and create, delete, or modify its animations using the Visualization Set Manager’s animation editor interface (as seen in Figure 4). When creating or modifying an animation, users can dynamically generate a preview of any frame in the data set by modifying the animation attributes and refreshing the preview’s image. In the case where VisIt is the selected rendering engine, this set of attributes includes the physical quantity, color table, range, domain, scale (e.g., linear, logarithmic, or skewed), and size of the animation in pixels. Flags can also be set to apply zone smoothing and to display the date that the source data was generated in the lower right hand corner of the animation. After the attributes of the animation have been saved, the altered visualization set is submitted to the server.

Once a CHIMERA simulation is transmitting output to Bellerophon, users can access the simulation’s visualization set with the Visualization Set Explorer tool. The first step is to select one or more sets using an instance of the visualization set selection user interface seen in the Visualization Set Manager, which allows sets to be filtered and sorted easily. The interface displays each visualization set’s index, unique id, creation date, and optional notes. In addition, information concerning the simulation - such as resolution, the number of the last frame produced, and the current physical time - is available. Once one or more visualization sets have been chosen, the Visualization Set Explorer provides robust access to its animations and provenance metadata. When an animation is selected, a small popup window populated with six options appears (see Figure 5). The user can load and play all animation frames in a viewer with VCR-like controls (see Figure 6); browse individual frames by loading them one at a time; create custom frames by modifying the animation’s attributes; download the MP4 movie; download a tar file consisting of the MP4 movie, all PNG images and the animation’s metadata (called a snapshot); or bookmark an animation of particular interest (called a hot

![Figure 5: A screenshot displaying various functions for accessing, viewing, customizing and downloading an animation.](image)
Users can also download the PNG image and source data file for the frame currently being viewed.

3 Software Engineering and Scientific Workflow Tools

In addition to data analysis, Bellerophon facilitates software engineering tasks for the CHIMERA development team [18]. Verification tasks are performed by an automated regression test system, which spans all components of Bellerophon’s n-tier architecture beginning with the supercomputing tier where programs attempt to checkout, compile, and execute the latest revision of CHIMERA every 24 hours. These results are transmitted to the web server where they are processed and then made available through the client-side Regression Test Explorer tool. When a test failure is detected, an email containing a hyperlinked stack trace is automatically sent to the responsible developers. These hyperlinks direct the developers to the file, line, and revision in CHIMERA’s online Trac repository browser [19]. Another tool, SVN Statistics On-Demand, allows users to execute the StatSVN code repository statistics generator [20] via Bellerophon’s web service over a custom date and/or revision range. StatSVN generates a set of interlinking HTML pages with tables and plots detailing statistical information about a project’s code development, including metrics like code churn and per-file heatmaps. Bellerophon addresses workflow management needs through the Important Links and Information feature. This client-side tool provides direct links to Trac’s source code browser for CHIMERA and the code’s public and private wikis, along with links to the OLCF, NICS, and NERSC homepages. With this tool, a user can also post to the CHIMERA mailing list, browse the mailing list archives, and create a new Trac ticket, as well as receive real-time status updates on OLCF, NICS and NERSC resources.

Figure 6: A screenshot of the Visualization Set Explorer animation viewer interface loaded with an animation of entropy data from a 512 x 256 CHIMERA 2D simulation with a 12 solar mass Woosley-Heger progenitor [18].
4 Utilization and Impact

The degree to which Bellerophon has become completely indispensable to the CHIMERA collaboration’s day-to-day work is its greatest triumph to date. Bellerophon has become the de facto work environment for development, regression testing, and analysis by the CHIMERA collaboration. All of the disparate members of the collaboration use Bellerophon on a daily basis for development and data analysis. This use occurs both in a collaborative mode, where several members examine a particular topic together, as well as in individual cases, where one person uses Bellerophon to produce a visualization artifact or test a new piece of code simply because it is the easiest environment in which to work.

Bellerophon’s data analysis capabilities are leveraged by the CHIMERA team in a myriad of ways. They provide collaborators the ability to monitor the progress of each simulation online. Users can keep tabs on important quantities such as current physical time, wall time, and cycle number. Bellerophon’s success as a debugger cannot be understated. Several insidious bugs and subtle runtime issues, which would have been difficult to deduce otherwise, have been discovered and isolated using these analysis tools. Usage metrics can also be calculated using Bellerophon. Important metrics, like wall time or physical time per run and throughput per platform, can be determined and used to plan future runs and allocation requests. Bellerophon also serves as the artifact manager for CHIMERA. Every data file processed by the system, along with its metadata and renderings, are accessible and tracked in Bellerophon’s database. This database now includes more than 25,000 Silo files, 350,000 PNG images, 60 continuously updated MP4 movies, and the complete results of over 2,200 regression tests.

5 Future Developments

Future enhancements to Bellerophon’s presentation tier include the development and deployment of Android tablet and phone apps enabling mobile access and control of Bellerophon. The mobile apps will allow users to text or email lightweight artifacts (e.g., images or plain text files) to collaborators, upload movies to a Bellerophon YouTube channel, and post updates to social media outlets such as Twitter. The next milestone concerning Bellerophon’s data analysis capability is an expansion to include the analysis of 3D results and generation of associated artifacts through the integration of visualization clusters into Bellerophon’s architecture. Given the sheer volume of CHIMERA 3D results, transmitting data over the network for rendering is simply unfeasible. This modification will also include an implementation of automated long-term storage of data (to, e.g., an HPSS repository). Finally, the generalization of Bellerophon to other HPC applications beyond the CHIMERA is well within sight. The first step in this generalization is to apply the system to GenASiS [21, 22], a computational astrophysics code under development at ORNL, and then on to other codes representing a variety of domains.

6 Conclusion

A software support system, Bellerophon, has been created over the past four years to facilitate the data analysis, software engineering and scientific workflow needs of the development team for CHIMERA, a multi-dimensional, multi-physics HPC code designed to study core-collapse supernovae. Bellerophon’s n-tier architecture integrates supercomputing resources at the OLCF, NICS, and NERSC facilities with a dedicated web and data server and a web-deliverable, cross-platform desktop application. This suite of easy-to-use online tools enables users of the system to
quickly view, in near real-time, animated 2D colormaps and lineplots of over a dozen physical quantities over time. The tools also allow users to robustly customize animations and to access and manage each simulation’s artifacts (e.g., source data, provenance data, images, and movies). Bellerophon assists with software engineering tasks by providing an automated regression test platform for CHIMERA. Now that an initial suite of tools has been developed, our next goal is to generalize the Bellerophon system to other codes and platforms.

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