AMP: A Science-driven Web-based Application for the TeraGrid

Matthew Woitaszek  
National Center for Atmospheric Research  
1850 Table Mesa Drive  
Boulder, CO 80305  
mattheww@ucar.edu

Travis Metcalfe  
National Center for Atmospheric Research  
1850 Table Mesa Drive  
Boulder, CO 80305  
travis@ucar.edu

Ian Shorrock  
National Center for Atmospheric Research  
1850 Table Mesa Drive  
Boulder, CO 80305  
ian.shorrock@gmail.com

ABSTRACT

The Asteroseismic Modeling Portal (AMP) provides a web-based interface for astronomers to run and view simulations that derive the properties of Sun-like stars from observations of their pulsation frequencies. In this paper, we describe the architecture and implementation of AMP, highlighting the lightweight design principles and tools used to produce a functional fully-custom web-based science application in less than a year. Targeted as a TeraGrid science gateway, AMP’s architecture and implementation are intended to simplify its orchestration of TeraGrid computational resources. AMP’s web-based interface was developed as a traditional stand-alone database-backed web application using the Python-based Django web development framework, allowing us to leverage the Django framework’s capabilities while cleanly separating the user interface development from the grid interface development. We have found this combination of tools flexible and effective for rapid gateway development and deployment.

Categories and Subject Descriptors

H.3.5 [Information Storage and Retrieval]: Online Information Services - Web-based services.

1. INTRODUCTION

In March 2009, NASA launched the Kepler satellite as part of a mission to identify potentially habitable Earth-like planets. Kepler detects planets by observing extrasolar transits—brief dips in observed brightness as a planet passes between its star and the satellite—that can be used to identify the size of the planet relative to the size of the star. However, in order to calculate the absolute size of an extrasolar planet, the size of the star must also be known. Asteroseismology can be used to determine the properties of Sun-like stars from observations of their pulsation frequencies, yielding the precise absolute size of a distant star and thus the absolute size of any detected extrasolar planets. The Asteroseismic Modeling Portal (AMP, http://amp.ucar.edu) presents a web-based interface to the MPIKAIA asteroseismology pipeline to a broad international community of researchers, facilitating automated model execution and simplifying data sharing among research groups.

While the MPIKAIA asteroseismology pipeline itself has been available to astronomers to download and run on their own resources for several years, its potential use for processing Kepler data provided compelling motivation to explore presenting the model as a science gateway. The most substantial barriers to an astronomer running the model on a local resource are MPIKAIA’s high computational requirements and straightforward but high-maintenance workflow. Running a single MPIKAIA simulation requires propagating several independent batches of MPI jobs and can consume 512 processors for over a week of wall-clock time. More importantly, the results of these asteroseismology simulations are of interest to an international community of researchers. Presenting the model via a science gateway allows researchers without local resources to run the model, disseminates model results to the community without repetition, and produces a uniform analysis of asteroseismic data for many stars of interest.

The straightforward workflow implemented by AMP also provided an opportunity to develop a new science gateway while exploring a new architecture, web application framework, and supporting technologies. One of the first steps when designing a science gateway is to select the collection of technologies, such as frameworks and toolkits, that will be used to construct the gateway. As noted by M. Thomas when similarly evaluating frameworks for science gateway development, gateways can be constructed using tools that vary greatly in complexity and features, with the most feature-rich frameworks often introducing substantial development complexity. Indeed, many of the prior science gateway projects at the National Center for Atmospheric Research (NCAR) followed the design pattern typical of many gateways by using Java to implement complex and highly-extensible service oriented architectures and web portals. Most notably divergent from our prior work, AMP does not use an application-specific service-oriented architecture and is not written in Java.

For the design and implementation of AMP, our objective was to create a web-based science-driven application that peripherally used Grid technologies to enable the back-end use of supercomputing resources. We prioritized minimizing development time and complexity while retaining full cre-
ative control of the user interface by selecting the Django rapid-development web framework and implementing the Grid functionality with command-line toolkit interfaces.

Due to AMP’s computational requirements, AMP has been designed since its inception to target TeraGrid resources. Many of the best practices and procedures for developing and deploying science gateways on the TeraGrid were proposed coincident with our initial exploration of targeting TeraGrid as AMP’s computational platform. As such, AMP also provides an example of constructing a new science gateway specifically for TeraGrid cyberinfrastructure rather than the common case of extending an existing gateway to utilize TeraGrid. AMP’s architecture separates the web-based user interface and the workflow system performing Grid operations, isolating interactive users both logically and physically from TeraGrid operations. We utilized only components common to all TeraGrid resource providers with the goal of facilitating easy deployment on current TeraGrid-managed resources without any resource provider assistance.

The remainder of this paper is organized as follows. Section 2 describes the asteroseismology model workflow and computational requirements. Section 3 and 4 describe the architecture, design, and implementation of AMP. Section 5 discusses our experiences with AMP’s implementation emphasizing the potential usefulness of the design principles for future gateway projects, and the paper concludes with continuing and future work.

2. BACKGROUND

The asteroseismology workflow provided by AMP consists of two components: a forward stellar model and a genetic algorithm (GA) that invokes the forward model as a subroutine. The forward stellar model is the Aarhus Stellar Evolution Code (ASTEC) 4, a single-processor code that takes as input five floating-point physical parameters (mass, metallicity, helium mass fraction, and convective efficiency) and constructs a model of the star’s evolution through a specified age. The output of the model includes observable data such as the star’s temperature, luminosity, and pulsation frequencies. In addition to the scalar parameter output, ASTEC produces data that can be used to produce basic graphical plots describing the star’s characteristics, including a Hertzsprung-Russell diagram showing the star’s temperature and luminosity and an Echelle plot summarizing the star’s oscillation frequencies.

In practice, however, the reverse problem must be solved: ASTEC models a star with known properties and produces its observable characteristics, while the real research product requires starting with observations and identifying the properties of a star that could produce those observations. In order to derive the properties of distant stars from observations, ASTEC is coupled with the MPIKAIA parallel GA 7 to create an automated stellar processing pipeline 7. The GA creates a population of candidate stars with a variety of physical parameters, models each star using ASTEC, and then evaluates each candidate star for similarity to the observed data. Over many iterations, the GA converges to an optimal candidate star that has the properties most likely to produce the observed data. The candidate star is then subjected to a solution detail run that further refines the star’s characteristics at a finer granularity and produces the final model output.

AMP supports both modes of execution from its web-based user interface: running the forward model with specific model parameters (a “direct model run”), and executing the GA to identify model parameters that produce observed data (an “optimization run”). Direct model runs are trivial to configure and execute: they require five floating-point parameters as input, take 10-15 minutes to execute on a single processor, and produce a few kilobytes of output. Optimization runs are both more complex and computationally intensive.

The optimization run workflow consists of an ensemble of independent GA runs, with each run requiring the execution of multiple sequential tasks (see Figure 1). For each optimization run, multiple separate GAs are executed and allowed to converge independently. Each GA (and indeed each task) is started with randomly generated seed parameters to encourage the GA to explore a wide parameter space, avoid local minima, and provide confidence in the optimality of the final result. The GAs can take from hours to days to converge depending on system performance and the number of iterations requested, so a GA may not converge in a single task execution within the target supercomputer’s walltime limitations. Thus, each GA run may require several invocations of the executable to converge to a solution. When all of the GA runs in the ensemble are complete, the best solution is evaluated using the forward model to produce detailed output for presentation and analysis.

In the current configuration for the Kepler data analysis, each optimization run consists of four GA runs executed in parallel, and each GA models a population of 126 stars (using 128 processors) for 200 iterations. One interesting artifact of the ASTEC model is that the execution time varies slightly depending on the target star’s characteristics. During the first few iterations, some stars in the randomly chosen population may take more time to model than others. Because the iteration is blocked on the completion of all stars in the population, the iteration run time is set by the longest-running component star. However, as the model continues and the population begins to converge, the model run time for each star also converges and the time to run each iteration decreases. Thus, the 200 iterations can be performed in about 160x to 180x of the first iteration’s measured time.

As part of the allocation request for TeraGrid resources, the stellar model was benchmarked on four TeraGrid platforms (see Table 1). From the astronomer’s perspective, the most important metric is the predicted optimization run (GA) run time. The modern Intel and AMD processors in the NICS and TACC resources can propagate the GA

![Figure 1: AMP asteroseismology workflow.](image-url)
to completion in about 40-60 hours, while the slower processors in NCAR’s Frost system can require over 12 days. When considering TeraGrid’s service unit (SU) charging factors and the model performance, the TACC systems are most efficient platforms for this model, but the systems are generally similar in cumulative charging. For our production deployment, we have targeted the NICS Kraken system due to its short solution time and support for WS-GRAM. The TACC systems demonstrated better performance, but the small disk space available on Lonestar and lack of WS-GRAM on Ranger, combined with the current allocation oversubscription on those systems, discouraged their use for this project. For additional computational volume, we continue to utilize NCAR’s Frost system.

### 3. Architecture

The high-level AMP architecture reflects our principal design goals of supporting rapid development and explicitly targeting TeraGrid computational resources. The architecture consists of three main components: the web-based user interface, the “GridAMP” workflow daemon that functions as a grid client, and the remote computational resources running the model (see Figure 2). The separation of these three main components is fundamental to the architecture.

With respect to supporting rapid development, one advantage of the separation of AMP’s functional components is its ability to support specialized labor. This approach generally decouples the tasks of web development, back-end Grid software engineering, and the debugging and maintenance of the science software itself. This is particularly beneficial because it is much easier to find students to work on web-related development (e.g., undergraduates) than to find students that possess a thorough understanding of the intricacies of Grid infrastructure and middleware (e.g., graduate students with several years of experience), to say nothing of trying to find students that can work proficiently (and efficiently) with both. Because the interface and Grid components are not tightly coupled, they can be easily developed and maintained by individuals with complimentary skill sets. We have continued the separation concept through to the science code itself by running the code in an environment identical to that used by the astronomy principal investigator and colleagues. Rather than dispatching software engineers or students to maintain the application, the science PI occasionally updates the Grid-executed code using `sudo` on the remote resource personally.

Separating the user interface from the grid-related processing components also simplifies the administrative responsibilities associated with using TeraGrid computational resources. In particular, one concern often associated with science gateways is their use of a shared credential to submit jobs on behalf of a community of individual gateway users [11]. Gateways that utilize TeraGrid resources are required to maintain user registries and associate every Grid request with a specific gateway user. In order to provide end-to-end user accounting for all gateway jobs and to allow resource providers to disambiguate the real users acting behind community credentials, TeraGrid has developed and deployed the GridShib SAML extensions [8]. However, an underlying risk remains: a science gateway typically runs a publicly accessible web server and also must possess the credentials necessary to access many machines on the TeraGrid.

The AMP architecture addresses this concern by separating users from the community account credential by placing them on distinct servers. The user interacts with a web portal located on one publicly-accessible server, while all back-end processing and remote Grid operations are performed by the GridAMP daemon on another server. All communication between the AMP portal and the GridAMP daemon are asynchronously performed by manipulating a database located on yet another server. Moreover, the roles and privileges of the public web portal and GridAMP daemon are strictly managed and controlled. The public web portal is essentially a database-driven web server without any Grid connectivity or Grid software. The server hosting the GridAMP daemon is accessible only to the developers using SSH keys, and only GridFTP is externally exposed to facilitate data staging via the Grid account credential. All input data from users is marshaled through the SQL database. Incoming user data is parsed by the web server and uploaded to database tables with strict data type constraints. When required, the input files are regenerated from the database by the GridAMP daemon and then staged to TeraGrid systems. It is thus exceptionally difficult to send any data other than a properly formatted astrometry input file to a TeraGrid resource, and even a full root compromise of the web server does not provide access to any credentials used for access to any other system. This architectural feature helps AMP comply at the most fundamental level with the TeraGrid science gateway security best practices [10].
4. IMPLEMENTATION

The AMP gateway and the GridAMP daemon are implemented in Python 2.4/2.6 using the Django web development framework [2]. Django’s primary intended use is as a web development platform, but over two software engineering iterations, we adopted Django as the underlying framework for both the AMP website and the GridAMP daemon. We were able to perform two complete cycles of a “spiral-model” software engineering process in about one year, completely re-implementing the entire website and processing daemon about 6 months after the initial prototyping commenced.

In our first development prototyping cycle, we perhaps took the separation of components concept too far, as we used Django to implement the website but implemented the GridAMP daemon in Python using manually-coded SQL database calls. This made sense at the time: although Django provides a full-featured object-relational model (ORM) independent of its web server-related features, we were skeptical that the ORM would be sufficiently robust to fulfill our requirements. For example, we demand direct and explicit control of the database schema and wanted to use database permissions to carefully control access to database tables on a per-user basis. Even the idea of allowing an ORM system to create tables based on Python object definitions seemed irreconcilable with production-quality science gateway implementation. Over the first six months of development, however, it became clear that this was not the case—the Django ORM was more powerful and flexible than we imagined could be possible. We were able to easily redefine our prior manually-specified database schema entirely using Django with perfect table/field/type correspondence, including our desired permissions scheme, all from within Django’s ORM. Moreover, the database schema could be reconstructed on demand—including sample data—in test databases when required for development work. The ORM also worked from standalone programs outside of Django’s web serving infrastructure.

Thus, the usefulness of the Django “don’t repeat yourself” philosophy quickly became apparent and immediately applicable to AMP. While the service separation philosophy can be taken to an extreme—we could have even switched languages between the web server and the GridAMP daemon—maintaining two separate codebases quickly became a mundane waste of time. We therefore maintained the operational separation of the web site and GridAMP daemon but unified the framework for both components. The entire project now uses a single code base to define and manipulate shared data structures across multiple servers.

4.1 Common Components

Software written with the Django framework is organized into “projects” and “applications”. A project basically represents a website and consists of a common configuration and a collection of installed possibly independent applications. Applications are written using the typical model-view-controller design pattern, better described as model-template-view using Django’s terminology. Models use the ORM to abstract database access behind Python objects while providing the opportunity to add custom functionality. When a HTTP request is received, the request is dispatched to the appropriate Python subroutine (a “view”) to perform necessary processing. View routines then usually conclude by rendering final output to the user via Django’s template engine.

For AMP, we implemented most of the science gateway functionality in a single core application consisting of ORM models and support routines. For example, the catalog of stars, their identifiers, the simulations, and the constituent supercomputer jobs are all stored in this core application. This effectively makes the most important components of AMP first-class global objects when imported properly. The web interface is then constructed of additional applications that refer to the core application as required. Only this core application’s models are shared between the website and the GridAMP daemon.

For both the web server and the GridAMP daemon, we also adopted Django’s built-in authentication “auth” framework. The authentication framework provides basic website user management functionality including common user-initiated account manipulation activities. We extended the Django authentication framework to support additional information required by AMP and TeraGrid, such as data provenance and user authentication metadata.

An additional benefit of using the Django ORM and authentication framework is that Django’s built-in development server provides an administrative interface that can manipulate ORM objects including those created by the authentication framework. The interface is also easily modified to support custom requirements. Thus, administrative tasks such as approving users or adjusting back-end parameters (like allocations and the authorization for a user to submit to a machine using a particular allocation) can easily be manipulated from a graphical interface without custom development. The interface is available to developers running the Django development server with appropriate database connectivity, so the administrative functionality is not even possible from any publicly accessible web servers.

4.2 User Interface

In addition to the shared Django application that contains the core AMP models, we wrote separate Django applications to implement independent portions of the website functionality. One application allows users to browse and search star catalogs, one allows users to view completed simulation results, and another facilitates simulation submission. These applications don’t contain models so they are useful only within the context of a Django project containing the core AMP application, but the distinction provided a logical separation of site components.

We also wrote additional standalone Django applications containing potentially reusable code. For example, we wished to use a CAPTCHA to reduce the possibility of automated bots requesting AMP accounts. Due to our accessibility requirements, using a typical image-only CAPTCHA was problematic, so we decided to write our own. Our general purpose question/answer CAPTCHA presents a series of questions with optional links to answers. For AMP, users are asked to enter the HD catalog numbers of popular stars, such as “What is the HD number for Alpha Centauri?” For astronomers that can’t remember, we present a link to the page containing the answer. With this, only one real estate agent turned fashion supernova has requested the ability to submit AMP jobs.

AMP’s web interface is quite typical for current database-driven websites in that it combines static and dynamic web
technologies to provide its user experience. AMP uses AJAX-based “Web 2.0” techniques to simplify the user experience where possible, but the site is fully functional without these JavaScript enhancements. For example, the process of searching for a star uses AJAX to suggest stars with results or in the Kepler catalog. If no stars are in AMP’s catalog, the search is passed to the SIMBAD astronomical database and the target, if found, is added to the local catalog. Finally, AMP uses Django’s SSL authentication and session management support to ensure that all activities performed by registered users is encrypted.

4.3 Grid Execution

To simplify the deployment of the AMP model on TeraGrid systems, we constructed a workflow that utilizes only basic components provided by the Coordinated TeraGrid Software and Services (CTSS) software stack. Rather than deploying a SOA with services that encapsulate the models as we have done in the past for other projects, the GridAMP daemon directly formulates and submits GRAM execution requests and GridFTP file transfers. Thus, the model can be deployed on a TeraGrid resource as soon as the community account has been authorized and no special resource provider dispensations (e.g., custom Globus containers or separate service hosting platforms) are required.

The remote resource execution environment for each AMP job is initialized and finalized using shell scripts invoked by GRAM using the fork job service. The pre-job stage creates a new empty copy of the model runtime directory structure and prepopulates the tree with static input files. The model is then run using GRAM through the scheduler interface with each model invocation staging in the small input data text file and staging out its restart progress file. The post-job stage uses tar to consolidate output and log files into a single file for transfer back to the GridAMP daemon and eventual delivery to the user via the website. A final cleanup stage ensures that the execution environment has been removed.

4.4 GridAMP Workflow Daemon

The GridAMP daemon manages the workflow of AMP simulations on remote grid resources. It reads simulation information from the centralized database, performs the necessary grid client actions, and updates the database accordingly. The AMP website and the GridAMP daemon thus interact asynchronously through the centralized database.

We wrote a custom Python module to handle the grid client functionality via calls to the Globus command-line interfaces. The module supports generating derivative proxy certificates with GridSHIB SAML extensions, GridFTP, and GRAM. The primary reason for using our own library was that we already had such functionality in-house and our familiarity with our grid support module made it seem simpler and more robust than using third-party solutions. The most important operational benefit for wrapping command line clients is that it provides excellent support for troubleshooting. The daemon produces logs that clearly highlight warnings and errors with the relevant command lines displayed for failure cases. To troubleshoot, a developer needs only to open a new console on the GridAMP server and copy-paste the line at the shell prompt to retry the failed action. The Grid operations are not hidden behind complex object models but are transparent so that problems can be investigated and corrected quickly and easily.

Due to AMP’s straightforward processing requirements, we also wrote our own workflow management daemon. The workflow is represented as a list of stages with function pointers that must return to proceed to the next state (see Listing 1). If the job is in a particular state, all of the functions in the subsequent list are called. If all return True, then the job is set to the indicated next state. In practice, the first function usually checks to see if the prior state has completed, and the last function propagates the job to the next state. This simple encoding can represent arbitrary trees of execution, but for AMP the processing is merely linear. The only coding cleverness is the use of inheritance to support AMP’s two job types with a single base class implementing all of the routine functionality. Job queuing, stage-in, and stage-out are all handled by the base class. Only the functions that generate the GRAM job definitions and perform model postprocessing are implemented in the derived classes. Thus, the derived classes are very small and contain only model-specific execution and postprocessing code.

Workflow state management and job status tracking are integrated with AMP’s data model as implemented using the Django ORM and stored in the centralized database. We utilized a two-level approach to workflow status management, integrating the simulation status in the application-specific data models while maintaining constituent grid job status in a more generic fashion. To manage the workflow, the daemon first polls the status of each grid job and updates the job records accordingly. This process is identical for all grid jobs regardless of purpose (pre-job, post-job, or simulation) or execution method (fork or queue), and no special callbacks or processing are performed as part of the grid job status update procedure. Once the grid job status has been updated, the workflow management code simply retrieves the last-known status of the appropriate job and waits or proceeds accordingly. One advantage to this approach is that simulation status is integrated at the highest level of the application-specific data model so the user interface does not need to analyze the state of many individual grid jobs to determine the current state of a simulation.

Listing 1: Example GridAMP workflow definition

```python
self.workflow = {
    'QUEUED': ( self.check_queued_sim, self.submit_prejob ),
    'PREJOB': ( self.check_prejob, self.submit_workjob ),
    'RUNNING': ( self.check_workjob, self.submit_postjob ),
    'POSTJOB': ( self.check_postjob, self.postprocess, self.submit_cleanup ),
    'CLEANUP': ( self.check_cleanup, self.close_simulation ),
    'DONE': ( ),
}
```
As part of the workflow management process, the GridAMP daemon also handles failures and provides user status notifications. Our error management philosophy completely isolates gateway users from the jargon of grid-related failures and transients. Users are not notified of events that they may not understand and are definitely not capable of correcting. Unless the asteroseismology model fails, the simulation will be completed and returned to the user. Users may opt to receive an e-mail when their simulation completes or to receive e-mails at each state transition.

The GridAMP daemon distinguishes between anticipated transients, model processing failures, and its own failures. Anticipated transients, such as remote systems suddenly becoming unreachable for GRAM or GridFTP requests, are handled silently: administrators are notified, the job’s status display is supplemented with a plain-text message describing the situation, and the processing is retried automatically without user or administrator intervention. Model failures, such as the absence of a mandatory output file or the failure of a result line to parse correctly, generally require gateway administrator intervention and occasionally escalate to the science investigators for model development work. In the event of a model failure, the simulation is moved to a special “hold” state and both the user and administrator are notified. The gateway administrators can then debug the problem and retry the failed processing steps interactively. Once the problem has been resolved, the workflow resumes automatically. Finally, failures of the GridAMP daemon itself are monitored externally and immediately brought to the attention of the gateway administrators.

5. DISCUSSION

Perhaps the most fundamental characteristic of AMP is its posture as a grid-enabled science gateway. When considering our earlier grid gateway projects and a small set of existing grid gateway frameworks, we realized that we did not really want to build a “grid gateway” in the sense suggested by these projects and frameworks. Rather, we wanted a science-driven web-based application focused on delivering the required functionality to our user community that happened to use grid resources and technology to perform some of its computationally intensive processing. To that end, AMP completely hides many aspects of its grid nature from users. As most astronomers are familiar with high-performance computing, concepts such as simulations, computational jobs, allocations, and supercomputers remain visible terminology, but the word “certificate” is not even mentioned anywhere on the site.

Our ability to decouple AMP’s front-end and back-end components was enabled by AMP’s straightforward workflow and lengthy job turnaround time. We recognize that the luxury of asynchronous coupling is not afforded by many science gateways that facilitate interactive analysis and visualizations. The decoupled asynchronous processing is appropriate for AMP’s jobs, simplified the implementation, and facilitates operational debugging.

While workflow management is well understood and a variety of robust technologies are available to automate workflows [1], it was indeed quite simple to implement a small-scale custom workflow manager for AMP. In fact, if GRAM ever supports executing pre-job and post-job scripts using the fork service as part of a queued job specification, half of AMP’s functionality could be implemented using a single GRAM job submission! For the optimization runs, the most complex portion of the workflow is downloading and interpreting partial result files, which requires custom implementation regardless of the workflow management paradigm. By writing our own simple workflow management daemon, we have retained a single application-defined representation of all state. The Django models used by the website are used for execution management by the GridAMP daemon. This avoids the need to deploy and query middleware to run grid jobs and provides the transparent end-to-end debugging capability that is useful when things go wrong.

We are particularly impressed with the Python-based Django web development framework. For our purposes, Django seemed to perfectly balance framework features and customization, supporting the rapid development web sites without being a content management system. The programming methodology was intuitive, suggesting but not enforcing a model-view-controller design pattern. The Django framework was useful even for the non-web portions of the project. The self-contained development environment was easy to install and facilitated quick prototyping and debugging. When combined with the Apache web server, the framework was robust enough to function as a production system.

Our use of AJAX and Web 2.0 technologies has been limited to cases where it is clearly beneficial to our user community. For example, the star search functionality suggests stars that are in the Kepler catalog and stars that have results as soon as a user types enough of a catalog identifier to disambiguate possible targets. Given the long job turnaround time, however, opportunities to make the website appear more dynamic are limited. We could do many cool tricks with AJAX and social networking, and it was very tempting to allow astronomers to “share a star” via Facebook or send simulation progress updates using Twitter. More pragmatically, we are currently working on using RSS feeds to allow astronomers to subscribe to stars of interest and adding dynamic links to astronomical catalogs and visualization services such as SIMBAD and Google Sky.

Although AMP was designed as a custom solution for a specific model and workflow, we believe that some AMP components may be a useful foundation for future similar grid gateway development. Of course, the AMP user interface is completely custom, but Django facilitates rapid web development in its own right. The core AMP models that represent jobs and the base classes of the workflow manager are potentially generic enough to support other applications and workflows with minimal changes. Although we have not done so, it would not be particularly difficult to isolate the common job management functionality from the models such that it could be added to new models as desired. The GridAMP daemon already supports this abstraction, as the workflow manager base class itself contains only grid code and all application-specific logic is contained in the workflow-specific derived classes. This level of abstraction would have to be similarly introduced to the data models by using complementary table schemas or inheritance to make a model represent grid jobs using a mechanism other than copying and pasting certain fields into the model definition. In this more generic approach, models would be defined only with application-specific job fields (such as input and results) with the job management fields provided externally. Thus, while AMP and its underlying components are clearly not a framework from which new gateways may eas-
ily be constructed, AMP demonstrates how rapid web development frameworks combined with simple grid support libraries can be used to produce useful science gateways.

6. FUTURE WORK

Although AMP is currently being used for friendly user testing and we do not anticipate making any fundamental changes over the next year or two, we have identified several front-end and back-end features that we wish to explore in the future. Again, we are currently investigating the best way to provide simulation progress and star result updates via RSS and refining our use of AJAX techniques to enhance the user experience in subtle yet meaningful ways. As the number of simulations on AMP grows, we anticipate that we will need to revisit the interface used to organize and present the results of the simulations.

One limitation of GridAMP that we intend to examine in the near future is its use of multiple sequential GRAM jobs to propagate optimization runs to completion. Although each GRAM job is set to the target system’s walltime (usually 6 or 24 hours), continuation jobs are only submitted once the prior job has finished. Thus, the continuation jobs must wait in the remote system’s batch queue before processing can resume. Many schedulers in use at TeraGrid sites support job chaining (or job dependencies) such that multiple jobs can be submitted at once and queued independently but declared eligible to run only after a prior job has completed. This would be perfect for AMP jobs, as the initial simulation submission could include the 4-8 jobs that are always required to perform the simulation, possibly reducing the cumulative queue wait time. We are currently making a graphical tool that plots job wait vs. execution time on a Gantt chart for each AMP simulation, as well as calculating aggregate execution wait and run time statistics, in order to understand the impact of queue wait time on various systems. We will then investigate Grid-based (but possibly nonstandard) methods to submit chained jobs on the resources at the providers that are the most tolerant of AMP’s computational workloads.

7. CONCLUSIONS

AMP has provided an opportunity to develop a new science gateway targeting TeraGrid computational resources. AMP’s straightforward workflow provided an ideal project to explore the use of the Python-based Django web framework for rapid prototyping and development of a science gateway. Our separation of the web interface, processing daemon, and science components simplified the system’s architecture and implementation. Furthermore, our use of common Django modules for both the web interface and the workflow daemon greatly reduced the complexity of implementation. The entire workflow was easily implemented using manual Globus command-line client calls to remote scripts and executables, further simplifying debugging and allowing AMP to be configured on remote resources without resource provider intervention. AMP is currently available for friendly user testing, and we anticipate the first extensive use of the system to perform new asteroseismology science using Kepler data in October 2009. In the future, we plan to examine possible applications of AMP’s architecture and underlying technology choices to other NCAR science gateway projects.

8. ACKNOWLEDGMENTS

We would like to thank to Nancy Wilkins-Diehr and the TeraGrid Gateways Program for assistance turning AMP into a TeraGrid science gateway. Stu Martin for assistance with Globus GRAM auditing, and Tom Scavo for assistance with GridShib. Thanks to Margaret Murray for helping us test GridAMP on TACC resources and to Victor Hazlewood and Rick Mohr for assistance with NICS resources. Paul Marshall performed the initial compilation and run time evaluation of MIPKAI A on several TeraGrid resources. Will Baird developed many prototype AMP components and features including AMP’s utilization of the SIMBAD [3] astronomical database. Michael Oberg prepared and manages the NCA RC Gateway Service Hosting Platform used to host AMP and GridAMP.

Funding to integrate AMP with TeraGrid resources was provided by the TeraGrid Science Gateways program. Computational time at NCAR was provided by NSF MRI Grants CNS-0421498, CNS-0420873, and CNS-0420985; NSF sponsorship of the National Center for Atmospheric Research; the University of Colorado; and a grant from the IBM Shared University Research program.

9. REFERENCES

[1] Condor Directed Acyclic Graph Manager (DAGMan). http://www.cs.wisc.edu/condor/dagman/
[2] Django. http://www.djangoproject.com
[3] SIMBAD Astronomical Database, CDS, Strasbourg, France. http://simbad.u-strasbg.fr/simbad/
[4] J. Christensen-Dalsgaard. ASTEC – the Aarhus STellar Evolution Code. Journal of Astrophysics and Space Science, 316:13–24, 2008.
[5] J. Cope, C. Hartsough, S. McCreary, P. Thornton, H. M. Tufo, N. Wilhelmi, and M. Woitaszek. Experiences from simulating the global carbon cycle in a grid computing environment. In Proceedings of the Fourteenth Global Grid Forum (GGF 14), Chicago, Illinois, June 2005.
[6] T. S. Metcalfe and P. Charbonneau. MIPKAI A – stellar structure modeling using a parallel genetic algorithm for objective global optimization. Journal of Computational Physics, 185:176–193, 2003.
[7] T. S. Metcalfe, O. L. Creevey, and J. Christensen-Dalsgaard. A stellar model-fitting pipeline for asteroseismic data from the Kepler mission. The Astrophysical Journal, 699:373–382, 2009.
[8] T. Scavo and V. Welch. A grid authorization model for science gateways. Concurrency and Computation: Practice and Experience, 2008.
[9] TeraGrid. Coordinated TeraGrid Software and Services (CTSS). http://www.teragrid.org/userinfo/software/ctss.php.
[10] TeraGrid. Security and Accounting for TeraGrid Science Gateways. http://www.teragrid.org/gateways/developers/security.php.
[11] TeraGrid. TeraGrid Gateway Security Summit. http://www.teragridforum.org/mediawiki/index.php?title=Gateway_Security_Summit, Jan. 2008.
[12] M. Thomas. Using the Pylons web framework for science gateways. In Grid Computing Environments Workshop, 2008. GCE ’08, pages 1–9, Nov. 2008.