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Workflow Management for a Cosmology Collaboratory

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Abstract

The Nearby Supernova Factory Project will provide a unique opportunity to bring together simulation and observation to address crucial problems in particle and nuclear physics. Its goal is to significantly enhance our understanding of the nuclear processes in supernovae and to improve our ability to use both Type Ia and Type II supernovae as reference light sources (standard candles) in precision measurements of cosmological parameters. Over the past several years, astronomers and astrophysicists have been conducting in-depth sky searches with the goal of identifying supernovae in their earliest evolutionary stages and, during the 4 to 8 weeks of their most "explosive" activity, measure their changing magnitude and spectra. The search program currently under development at LBNL is an earth-based observation program utilizing observational instruments at Haleakala and Mauna Kea, Hawaii and Mt. Palomar, California. This new program provides a demanding testbed for the integration of computational, data management and collaboratory technologies. A critical element of this effort is the use of emerging workflow management tools to permit collaborating scientists to manage data processing and storage and to integrate advanced supernova simulation into the real-time control of the experiments. This paper describes the workflow management framework for the project, discusses security and resource allocation requirements and reviews emerging tools to support this important aspect of collaborative work.

1. Introduction:

In the next 5 years the Nearby Supernova Factory at LBNL will increase both the quantity and quality of observational supernova data at low redshift by several orders of magnitude. The purpose of these experiments is to improve the use of supernovae as a tool for cosmology by determining the underlying physics behind these catastrophic events and then utilize this tool to help us understand the dark energy that drives the acceleration of the universe. These high quality observations will allow us to put tight constraints on the progenitors of supernovae, their luminosities, explosion mechanisms and any potential evolutionary effects which might bias the determination of the cosmological parameters.

Several aspects of the SNFactory set it apart from other supernova experiments. Foremost among these is that supernovae will be discovered using a blind wide-area CCD-based survey; other nearby supernova projects target known galaxies but there is now evidence that this approach misses an important subset of supernovae. In addition, the SNFactory will coordinate discovery and follow-up observations, eliminating delays and spotty early lightcurve coverage. It is expected that with the SNFactory detailed follow-up of supernova candidates can begin within as little as 12 hrs of the discovery observations. Finally, SNFactory follow-up observations will use an integral field unit spectrograph, data from which can be used to construct both detailed flux-calibrated spectra and broadband images. The regular photometric spectral time series for nearby supernovae the SNFactory will revolutionize the study of supernovae.

The data from the SNFactory will also be crucial for the study of the nuclear processes in supernovae using detailed simulation. The development of accurate models requires a detailed comparison with supernova data. This work will compare supernova light spectra over the full light curve. This gives an unparalleled view into the heart of a supernova as each layer in turn becomes transparent. The result is, in effect, a tomograph of the nuclear explosion.

2. The Nearby SNFactory:

There are two major components of the program, discovery and follow-up. The SNFactory will search for supernovae using CCD images obtained by JPL's Near Earth Asteroid Team (NEAT) using a 1.2-m telescope on Haleakala, Hawaii. NEAT's frequent sky coverage gives the SNFactory the potential to find thousands of supernovae shortly after they explode. In addition, since this search covers large portions of the sky irrespective of known galaxies, it will be rid of the biases to which pointed searches are subject due to their reliance on existing galaxy catalogs. NEAT will soon quadruple its capacity, with a second 1.2-m telescope operating at Mt. Palomar with a large CCD camera. NEAT data (up to 80 Gbyte/night) will be transferred in near real-time via high-speed Internet connection to LBNL/NERSC. Once there, the images will be processed and searched using automated software.

The most revolutionary aspect of the SNFactory -- aside from the huge numbers of supernovae it will find -- is the coordinated follow-up using instrumentation tailored to the study of supernovae. Candidate supernovae found in the NEAT images must first be screened with spectroscopy to confirm the supernovae and reveal its type (Ia, II, Ib, Ic) and redshift. The SNFactory will not only discover supernovae closer to explosion that other surveys and it will also begin the follow-up much sooner.

3. Computer Science Requirements:

We are designing a collaborative computing environment that provides the infrastructure and services necessary to manage the scientific workflow and user interactions for present and future large-scale supernova searches and to allow integration of these experiments with supernova simulation efforts. Large quantities of data from wide-field, ground-based telescopes will be processed each night to discover new supernovae. These supernovae will then be analyzed in real-time to determine which ones will be targeted for follow-up. During and after the follow-up data have been obtained, theoretical simulations of both the light curves and spectra of the supernova will be carried out on the NERSC supercomputers and clusters in order to further our understanding of these objects and their role in determining the cosmological parameters. The modeling will also be used to validate various aspects of our understanding of the supernova mechanisms and their progenitors. Both of these in turn will lead to a new set of priorities for our target list of supernovae that require follow-up.

Successful operation of such an undertaking requires a software environment that couples long-term control and monitoring of the data acquisition and analysis activities with tools that facilitate daily communications and interactions between widely distributed collaboration members located at sites worldwide. Furthermore, successful operation of future supernovae search programs will require that this design be scalable to accommodate future increased scope.

The use of automated workflow management will have a major impact on the study of supernovae and on the use of supernovae for cosmology. To improve the quality of supernova data early discovery and classification are crucial and will be improved dramatically with automated workflow. In addition, the use of simulations to guide the follow-up will ensure that the data taken are optimally timed for each type of supernova. The availability of high quality spectra will permit detailed comparisons between simulations and observations. This will allow scientists to develop full 3D simulations that include all known nuclear physics and accurately model a wide variety of real supernovae.

4. Computational Grids:

The availability of computing grids presents a unique solution for the computing challenges found in the SNFactory and will provide a strong, supportable basis for its implementation. To this end, we have already begun the process of implementing portions of the supernova search analysis code on the prototype Science Grid system under development at the LBNL NERSC facility. Within the grid environment, one of our first tasks will be to extend the current security environment to include remote sites involved in both supernova simulation studies and observation activities. While some mechanisms for allowing secure remote access to grid resources are already in place, this project will require extensions to these models, particularly in the area of secure high-speed data transfer. We will also need to explore the security and trust boundaries between centralized grid resources and other non-grid collaboration systems. And lastly, given the production nature of the computing environment we are creating, we will have ample opportunity to exercise grid security policies and implementations and lobby for those services that are most effective and efficient.
A key component of the computing grid infrastructure is its directory-based information service. The SNFactory, with its dependence on external data sources (observatories) as well as distributed compute and storage resources, will require automated, run time mechanisms for discovering and accessing a wide variety of these resources. We expect to develop, implement and test our resource model through the extensive use of grid information services. A coherent and long-lived system design must be based on an abstract representation of computing and system services that will be operational at least as long as the project itself. Grid technology represents just such an abstraction.

5. Workflow Frameworks:

Overlaying this distributed environment will be a data analysis effort that, at least initially, will rely on human intervention of collaboration members to train supernova search algorithms and verify their correct operation. Given the continual flow of observational images and the need to feedback observational instructions, this computing environment must operate in a mode of continuous daily production. During this same period, researchers will be simulating new data models in an attempt to match and subsequently direct further observations. At the operational level, the system design must also accommodate differences between resource access and allocation mechanisms will differ between search-dedicated systems and those used at production scientific computing facilities, namely NERSC. Furthermore, these differences extend to very practical issues such as responsibility for system availability and the scheduling of planned resource outages (e.g. HPSS) which are distributed among multiple administrative organizations.

Software systems that provide tools for defining and controlling overall process execution in this step by step fashion are collectively referred to as workflow management frameworks. While many workflow frameworks have been developed, some commercially, few have been successfully applied to the problem of managing scientific data analysis. One obvious reason has been the software industry focus on profitable applications in the business domain. However, an additional factor has been that workflow systems are most amenable to processes that are well understood and characterized (i.e. "engineered processes"). While this is often not the case in small, short-lived research efforts, supernova search programs with their extensive data processing needs and long-term operations are an excellent match for these systems.

6. Implementation:

Based on the present state and evolution of commercial tools and the availability of suitable building blocks within the grid development community, we will provide a set of workflow management services specifically aimed at the DOE Science Grid computing environment. We will provide job submission, tracking and completion notification services through a SWAP-based (Simplified

Workflow Access Protocol) workflow engine. This service will allow browser and program-based job submission and job tracking services across the entire collaborative computing environment. By integrating this service with existing grid security services, we can provide a secure, distributed control environment for data analysis operations. At a higher level, these services will ultimately be integrated into a collaboration-specific, standards-based workflow manger that contains descriptions of all data transfer and analysis sequences used during daily operations. We believe this approach will allow the early automation of both simple task sequences as well as allowing future implementation of generalized problem solving environments.

Most actual computing tasks required during analysis and categorization of sky image data execute as what is commonly described as “trivially” parallel tasks. While viewed, at the highest level, as simple tasks (e.g. “analyze tonight’s sky images”), they decompose into a varying set of data transfer and analysis tasks that each require their own job submission, tracking and exception handling services. Furthermore, the ability to allow these parallel tasks to “expand” into a set of computing resources that can vary in both equipment availability and usage authorization policies requires complex interactions between the workflow manager and grid information and authorization services. Therefore, we plan to incorporate the Condor distributed, high throughput computing software architecture into our workflow engine application. Several key features of the Condor architecture are important to the implementation of a workflow manager within the grid-computing environment. First, the Condor system has been designed to operate reliably and predictably in highly distributed environments. As a result, it fits well into the DOE Science Grid environment. Second, it contains an integral publishing scheme (“Class Ads”) that provides a flexible mechanism for matching job requirements to available computing and storage resources. And lastly, within the Condor package, there lies a parallel execution job manager, DAGman (Directed Acyclic Graph job manager) that can schedule parallel job execution on available resources as constrained by a tree-like dependency description.

As noted earlier, an effective workflow manager must have a persistent view of both the overall process and the state of all individual portions of that process. Most commercial workflow management packages rely on a central relational database server for retaining both the overall process description and the state of individual process steps. Given the highly distributed nature of the grid-computing environment, we feel that this approach creates problems in both the area of system scaling and system administration. We intend to encode process execution request and state information within XML encoded documents and have them stored within WebDAV-enabled (Web-based Distributed Authoring and Versioning) web servers. This choice is based on both our current positive experience with both WebDAV client and server software packages and it’s incorporation into the SWAP workflow reference standard.

A successful design for automating large scale computing tasks must include mechanisms for detection, notification, and rescheduling of jobs when such errors are encountered. Therefore the same interface that provides a persistent interface for job submission and state information will also allow process designers to specify actions to be initiated on encountering various classes of exceptions. It should be noted that propagation of these error conditions from individual execution nodes to a high-level workflow manager requires an effective global event distribution system. We share this requirement with many other grid-based software development projects and will be working closely with Grid Forum working groups currently addressing this issue and anticipate using a common, well supported event notification service within our workflow manager implementation.

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