

Large Synoptic Survey Telescope (LSST)

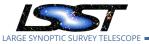
Data Management Middleware Design

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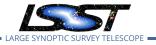
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Abstract

The LSST middleware is designed to isolate scientific application pipelines and payloads, including the Alert Production, Data Release Production, Calibration Products Productions, and science user pipelines executed within the LSST Science Platform, from details of the underlying hardware and system software. It enables flexible reuse of the same code in multiple environments ranging from offline laptops to shared-memory multiprocessors to grid-accessed clusters, with a common I/O and logging model. It ensures that key scientific and deployment parameters controlling execution can be easily modified without changing code but also with full provenance to understand what environment and parameters were used to produce any dataset. It provides flexible, high-performance, low-overhead persistence and retrieval of datasets with data repositories and formats selected by external parameters rather than hard-coding. Middleware services enable efficient, managed replication of data over both wide area networks and local area networks.



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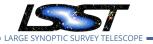
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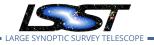
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1 Introduction

This document describes the baseline design of the LSST data access and processing middleware, including the following components:

- Data Backbone
- Data Butler Access Client
- Task Framework
- Workload/Workflow Management
- Processing Control

The Data Backbone manages the storage of LSST data products. The Data Butler Access Client provides a flexible interface for retrieving and persisting those data products. The Task Framework defines how scientific algorithms are packaged into pipelines, including how they are configured, how they use the Data Butler to access data, and how they execute on multiple nodes or cores. Workload and Workflow Management interfaces with the Task Framework to sequence the execution of dataflow graphs across one or more distributed computational environments. Processing Control uses the Workload and Workflow Management tools to execute campaigns (applications of pipelines with specific configurations to sets of data) in an efficient, fault-tolerant manner while monitoring the state of execution.

Common to all aspects of the middleware design is an emphasis on flexibility through the use of abstract, pluggable interfaces controlled by managed, user-modifiable parameters. In addition, the substantial computational and bandwidth requirements of the LSST Data Management System (DMS) force the designs to be conscious of performance, scalability, and fault tolerance. In most cases, the middleware does not require advances over the state of the art; instead, it requires abstraction to allow for future technological change and aggregation of tools to provide the necessary features.

Requirements for the DMS Middleware are defined in LDM-556.

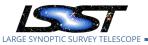


Figure 1 illustrates how various parts of the middleware interact with each other.

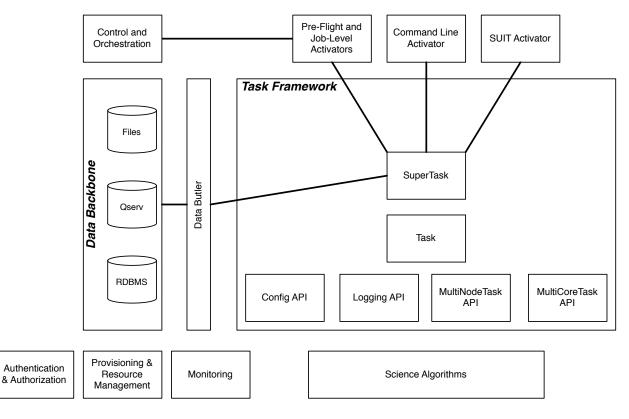


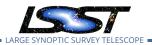
FIGURE 1: Data Management Middleware and Infrastructure

2 Data Backbone

The Data Backbone (DBB) provides data management (storage, tracking, and replication) for LSST data products that reside in non-computational storage tiers. It provides policy-defined operations for intra-site and inter-site data distribution, access latency requirements dependent upon the lifecycle of the data, data protection and recovery, data retention and eviction given cadences and predicted and observed on-demand usage, and efficient bulk recall of data which are spatially, temporally, or otherwise related in support of processing or export. See Figure 2.

The Data Backbone serves as an abstraction against storage components whose similar requirements may otherwise have been met through duplication of effort during construction and operations. From the perspective of data producers and consumers, the Data Backbone provides a common, well-defined concept of how all participating storage components are

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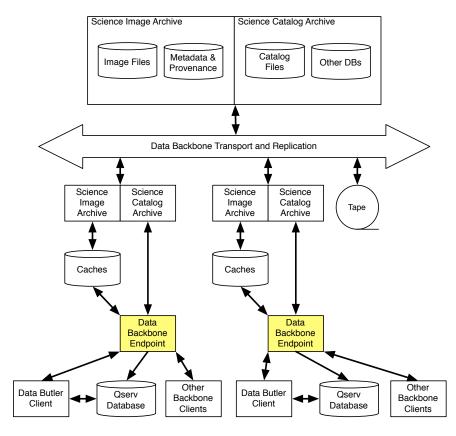


FIGURE 2: Data Backbone



expected to function, which greatly simplifies understanding of the system as opposed to understanding differing personalities of a large number of components.

The Data Backbone links all of the computational enclaves and the Data Access Centers, acting as the spine that supports them all.

Rucio [14] is being considered as an overall DBB system for files.

Replication and Transport 2.1

The Data Backbone spans the Base Site, Archive Site, all Data Access Centers and all sites participating in annual data release processing. Data products can enter the Data Backbone at any location as permitted by policy and are subject to timely distribution, access-latency guarantees, and eviction as defined by the policy. The Data Backbone provides data protection of data products while resident with the backbone.

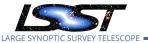
Movement operations supported by the Data Backbone include:

- Staging: data is copied in and out of the Data Backbone in coordination with an external management system; primarily used for workflow orchestration.
- Caching: data location and lifetime is managed by policy; caches are populated by use.
- Mirroring: 1:1 replication of data is dictated by policy.
- Export: data is copied out of the Data Backbone to end users;

The Data Backbone does not include public access restrictions, responsibilities regarding proprietary data periods or users with data access rights, or authorization or authentication of external users or services. This functionality is provided by layers on top of the Data Backbone, in the LSST Science Platform (LSP), Identity Management, and Bulk Distribution components.

Tiers within the Data Backbone include a custodial store with assurance of data preservation (e.g. tape but possibly other technologies) and an access tier that may have lower latency.

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Replication between sites and transfer to the custodial store is currently envisioned to be handled by layered utilities, so the DBB does not necessarily present a single-filesystem view. File transport technologies such as Globus Transfer [4] with GridFTP and RESTful interfaces are being considered.

2.2 Location and Metadata

The Data Backbone tracks the locations of all replicas of data ingested into it, along with their metadata and provenance. This information is stored in global, replicated database tables that are part of the DBB.

2.3 Files

The Data Backbone holds all files that are part of the Science Image Archive, including raw data and processed data products, as well as additional files such as the Engineering and Facilities Database Large File Annex, files associated with the Calibration Database, etc. It is also currently envisioned to contain files representing the archival contents of the catalog data products, either canonical files that are ingested into database servers or backup files dumped from canonical databases.

These files will be kept on a high-performance, scalable file store and archived in a reliable long-term file store. The baseline design uses GPFS [3] and HPSS [5], but drawbacks to these have been identified. Investigations of alternate storage technologies such as object stores (including Amazon Glacier [1]), Campaign Storage [2], and Quobyte [12] have been performed, but future work remains in this area.

2.4 Databases

The Data Backbone holds many databases that are part of the Science Catalog Archive that is visible to data rights holders. Exceptions are currently envisioned to include the largescale Data Release (Level 2) catalogs that are loaded only into the Qserv software described separately in LDM-135, which are considered as outside the Data Backbone. The associated metadata will be part of the Data Backbone, even if it is also replicated into the Qserv software. The Calibration Database, the transformed Engineering and Facility Database, and the (external-facing) Level 1 Database are all currently envisioned to be part of the Data Back-





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bone.

Just like files, these databases need to be managed in terms of replication, disaster recovery, and lifetime. The underlying mechanisms for data storage and transport and the interfaces to the data are significantly different, however. Accordingly, all databases are stored in appropriate database management systems that provide their own native mechanisms for replication and backup. These include an "off-the-shelf" relational database server (for which MySQL/MariaDB [8], Oracle [10], and Microsoft SQL Server [15] are being evaluated). A large instance of such a server is currently envisioned to be used as a "consolidated" database management system containing science data, metadata, provenance, and production tracking information, particularly for Level 2 Data Release Production. Additional databases such as the internal, Alert Production-only Level 1 database containing DIAObjects, DIASources, and DIAForcedSources; tracking information for the Level 1 Image Ingest and Processing system; or measurements for the Quality Control systems may reside in their own specialized storage outside the Data Backbone.

2.5 Interfaces

The primary access to the Data Backbone files is currently envisioned to be via mounted POSIX filesystems, but additional web service methods for retrieving files are contemplated.

The primary access to the Data Backbone databases is via direct queries to the relevant database servers. For portability and future-proofing, such queries should typically be intermediated with a package such as SQLAlchemy so that the underlying database software can be changed.

An ingest utility will transfer files into the Data Backbone and load their metadata and provenance into the appropriate DBB database tables. No file will be made available to be retrieved before its contents and metadata are complete. (It may be possible for file metadata to exist without file content if the fact that content does not yet exist or will never exist is recorded and made available along with the metadata.)

Since the DBB file metadata tables are large, complex, and hosted on a consolidated database server instance, their service level is not currently envisioned to be guaranteed to be high enough to directly support observatory operational processes. Accordingly, ingestion of raw data from the LSSTCam, ComCam, and Auxiliary Telescope Spectrograph occurs from the

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Observatory Operations Data Service, which can maintain a higher level of availability and therefore act as an ingest buffer.

Batch worker nodes should not expect to have direct access to DBB filesystems or the DBB databases. While exceptions could be made, none are currently envisioned.

LSP instances, including Portal, JupyterLab, and Web API nodes, will have access to DBB filesystems (either through mounts or through web services) and direct client access to DBB databases.

Since Science Pipelines codes will need to run in multiple environments including both batch worker nodes and LSP instances but also including development environments, they use the Data Butler (Section 3) to isolate themselves from the details of access interfaces.

Data Butler Access Client 3

This component is the framework by which applications retrieve datasets from and persist datasets to file and database storage. It provides a flexible way of identifying datasets, a pluggable mechanism for discovering and locating them, and a separate pluggable mechanism for reading and writing them.

3.1 Key Requirements

The framework must provide persistence and retrieval capabilities to application code. Persistence is the mechanism by which application objects are written to files in some format or a database or a combination of both; retrieval is the mechanism by which data in files or a database or a combination of both is made available to application code in the form of an application object. Persistence and retrieval must be low-overhead, allowing efficient use of available bandwidth. The interface to the I/O layer must be usable by application developers. It is required to be flexible, allowing changes in file formats or even whether a given object is stored in a file or the database to be selected at runtime in a controlled manner. It must be possible to store image pixel data in a file while part or all of its metadata is stored in a different file or in a database table.

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3.2 Baseline Design

The framework is designed to provide access to datasets. A dataset is a logical grouping of data that is persisted or retrieved as a unit, typically corresponding to a single programming object or a collection of objects. Datasets are identified by a set of key/value pairs along with a label for the type of data (e.g. processed visit image). Datasets may be persisted into multiple formats.

The framework is made up of two main components: a "Mapper" that manages cameraspecific repositories of datasets and determines the logical location of an identified dataset and a "Butler" that performs persistence and retrieval for that dataset. In the baseline design, the Butler wraps the Mapper and provides the exposed interface; it is anticipated that future evolution will increasingly separate these two. Both components are implemented in Python.

The Butler and its included Mapper manage repositories of datasets which can be in files or in a database. Operations on datasets include get, put, list, and check for existence.

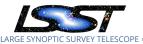
The Butler contains a pluggable set of serializers that handle persistence to and retrieval from serialization formats such as Python pickle files, task configuration override files (Python scripts), and FITS tables; separate plugins handle different types of storage such as filesystems, object stores, or SQL databases.

The Butler is initialized with zero or more read-only input repositories and one or more read-/write output repositories. When reading a dataset, the output repository is searched first; the "chained" input repositories are searched if the dataset is not found. When writing a dataset, the dataset always goes to the output repository, never to the chained inputs (unless the output is specified as being the same as an input). The set of input repositories is recorded for provenance purposes and for future uses of the output repository.

The Mapper translates from a dataset type name and one or more astronomically meaningful key/value dictionaries into a dataset location and storage. The location might be a pathname or URL for a file; it would include an SQL query for a database.

The Mapper provides flexibility at many levels. First, it allows the provided key/value dictionaries to be expanded using rules or database lookups. This can be used to map from a visit identifier to an exposure length, for example, or from a CCD name to an equivalent num-

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ber. This facility is used to implement the "rendezvous" of raw data with its corresponding calibration data. Second, it allows the key/value pairs to be turned into a location string using a dataset type-dependent method. Typically, this will be performed by substitution into a dataset type-specific template. Third, the Mapper allows camera-specific and repository-specific overrides and extensions to the list of rules and templates, enabling per-camera and dynamic dataset type creation.

For LSST, the Mapper flexibility is used in several ways. For precursor data, image files can retain the names they were assigned in the upstream archive, with templates being used to compute the filename from the values in the dictionary. Metadata stored in a SQLite database within the repository allows more rapid listing of available datasets and expansion of partial key/value dictionaries. Calibration data is associated with images by observation timestamp using validity ranges stored in an auxiliary SQLite database. For LSST Data Release Production, the same mechanisms will be used to process data staged from the Data Backbone (DBB). Direct access by the Data Butler to the Data Backbone (e.g. from the LSST Science Platform) will use DBB metadata tables directly. The Mapper will produce logical file identifiers that the DBB converts to endpoint-local physical locations. For LSST Alert Production, the Mapper will be configured to point to raft images on the distributor nodes and locally-cached calibration and template images.

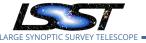
3.3 Alternatives Considered

Use of a full-fledged object-relational mapping system for output to a database was considered but determined to be too heavyweight and intrusive. Persistence from C++ was tried and found to be complex and unnecessary; Python persistence suffices since all control is in Python.

3.4 Implementation

A Python implementation of the design has been in place since DC3 prior to Final Design Review. This implementation has evolved substantially since then to simplify the pluggability of serialization and storage, to simplify the configuration of common Mapper subclasses, to allow and maintain more repository configuration information within the repository, to support multiple input and output repositories, to provide a configurable (rather than hardcoded) mechanism for retrieving and persisting composite datasets that are made up of more

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than one serialized dataset, to replace a custom configuration file format with standard YAML [16], and to provide support for caching persisted and retrieved objects in memory.

Since low-level serialization code is implemented in C++ or external libraries, I/O performance remains good.

4 Task Framework

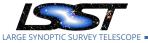
The Task Framework enables the packaging of scientific algorithms into executable and reusable pipelines. It handles configuration, argument parsing, and interfacing with the I/O and interprocess communications mechanisms.

The Task Framework is a Python class library that provides a structure of standardized class entry points and conventions to organize low-level algorithms into potentially-reusable algorithmic components called Tasks. Sample Tasks might include dark frame subtraction, object detection, or object measurement. The Framework organizes tasks into basic pipelines called SuperTasks. Sample SuperTasks might include processing a single visit, building a coadd, or differencing a visit. The algorithmic code is written into (Super)Tasks by overriding classes and providing implementation for standard entry points. The Task Framework allows the pipelines to be constructed and run at the level of a single node or a group of tightly-synchronized nodes. It allows for sub-node parallelization: trivial parallelization of Task execution, as well as providing parallelization primitives for development of multi-core Tasks and synchronized multi-node Tasks.

The Task Framework serves as an interface layer between orchestration and the algorithmic code. It exposes a standard interface to Activators (command-line runners as well as the workflow component and automated QC systems), which use it to execute the code wrapped in Tasks. The Task Framework does not concern itself with fault-tolerant massively parallel execution of the pipelines over multiple (thousands) of nodes nor any staging of data that might be required; this is the concern of the orchestration and workflow middleware.

The Task Framework exposes to the workflow system the needs and capabilities of the underlying algorithmic code (i.e., the number of cores needed, expected memory-per-core, expected need for data). It may also receive from the orchestration layer information on how to optimally run the particular task (i.e., which level of intra-node parallelization is desired).

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4.1 SuperTask

A SuperTask represents a unit of (generally transformational) work to be performed on data. Its primary responsibility is to provide the interface between Activators and Tasks. In doing so, it separates input and output from computation, making Tasks more reusable and enabling data movement and other optimizations within a distributed execution environment. The SuperTask also exposes the kinds of data that it accepts and generates. For example, a coaddition SuperTask might operate on a set of processed visit images and produce a patch of a coadded image. The specific data items to be processed are supplied through the Activator-SuperTask interface. The goal of the design is that any SuperTask can be run in any computational environment, from a laptop command line to the large-scale Data Release Production.

In general a SuperTask receives the content of its inputs and produces its outputs by invoking the Data Butler.

The SuperTask base class is a subclass of Task. This is so that SuperTask can take advantage of the configuration mechanism for Tasks. The hierarchy of Tasks in a specific application therefore extends all the way up to the top-level SuperTask, and each level is addressable for configuration discovery and overrides.

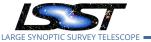
Each SuperTask implements a method that groups the input datasets into "quanta" that are the minimal units of work for an instance of the SuperTask and notifies the Activator of the outputs to be produced from each such unit of work. It also implements a method to execute a computation on a single quantum of data, typically by retrieving the inputs from the Data Butler and executing the underlying Task, followed by persisting the outputs, again using the Data Butler.

Datasets, as with the Data Butler, are specified by a set of key/value pairs, typically obtained by performing a database query on metadata tables, along with a label for the type of data (e.g. processed visit image).

SuperTasks also expose their processing requirements to their Activators, such as a need for multi-node communication or multi-core execution.

SuperTask implementation is in the prototype stage. The previous design and implementation combined the Activator and SuperTask functionality into a single class (CmdLineTask) that

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is now being replaced.

4.2 Activators

The Activator is responsible for providing a Butler instance for the SuperTask's use. It is also responsible for instantiating the SuperTask to be run and for providing necessary inputs to the configuration parameter mechanism (see section 4.4) for the SuperTask. For example, the "command line Activator" identifies the SuperTask to be run by name, locates and instantiates it, and provides for command-line overrides of config parameters of the SuperTask. It also creates a Butler based on one or more provided or defaulted data repositories.

An Activator is responsible for arranging for the execution of a SuperTask's execution method one or more times over a set of dataset specifiers. Via collaboration with the SuperTask interfaces, the Activator is able to determine the parallelization and scatter-gather behavior that is permissible and/or required to implement the workflow defined by the SuperTask.

The Activator therefore controls the input/output data access environment as well as the computational environment of the SuperTask. It is the plugin that enables SuperTask portability and reuse.

Specific Activators that are part of the design include a command line Activator and a workflow Activator that can be used to determine the data needed and produced by a SuperTask before its execution in order to configure data staging capabilities.

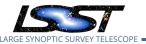
Activator implementation is in the prototype stage.

4.3 Task

Tasks are simply Python scripts with a common base class. Using Python enables Tasks to support complex control flows without developing a new control flow language. Tasks may hierarchically call sub-Tasks as part of their execution. Errors are reported through standard Python exception subclasses.

Tasks provide by default three facilities commonly used by all algorithmic code: configuration, metadata, and logging. The Task base class provides configuration facilities using the config-

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uration framework. The Task configuration can include selection of sub-Tasks to be executed, allowing the pipeline to be reconfigured at runtime. The Task class allows Tasks to save metadata related to their processing, such as performance or data quality information, separate from their data products. Each Task provides a default logger instance associated with the Task's name and position within the Task/sub-Task hierarchy.

The basic Task implementation is complete and resides in the pipe_base package.

4.4 Configuration

The configuration component of the Pipeline Framework is a mechanism to specify parameters for applications and middleware in a consistent, managed way. The use of this component facilitates runtime reconfiguration of the entire system while still ensuring consistency and the maintenance of traceable provenance.

4.4.1 Key Requirements

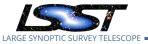
Configurations must be able to contain parameters of various types, including at least strings, booleans, integers, and floating-point numbers. Ordered lists of each of these must also be supported. Each parameter must have a name. A hierarchical organization of names is required so that all parameters associated with a given component may be named and accessed as a group.

There must be a facility to specify legal and required parameters and their types and to use this information to ensure that invalid parameters are detected before code attempts to use them. Default values for parameters must be able to be specified; it must also be possible to override those default values, potentially multiple times (with the last override controlling).

Configurations and their parameters must be stored in a user-modifiable form. It is preferable for this form to be textual so that it is human-readable and modifiable using an ordinary text editor.

It must be possible to save sufficient information about a configuration to obtain the value of any of its parameters as seen by the application code.

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4.4.2 Baseline Design

The initial design based on a custom text file format has been refined based on experimentation during the design and development phase.

Configurations are instances of a Python class. The class definition specifies the legal parameter names, their types, default values if any, minimum and maximum lengths for list values, and whether a parameter is required. It also mandates that a documentation string be provided for each parameter. Use of Python for defining configurations enables inheritance, the use of package imports to easily refer to configurations from other components, complex parameter validation, and the ability to define powerful new parameter types. Default values in configuration instances can be overridden by human-readable text files containing normal Python code, simplifying the specification of multiple similar parameters. Overrides can also be set using command line parameters. The Python base class maintains complete history information for every parameter, including its default and all overrides. The state of a configuration as used by the application code can be written out and optionally ingested into a database for provenance purposes .A mechanism is provided to automatically translate between the Python configuration instance and a control object for C++ code.

4.4.3 Implementation

An implementation of the Python-based design in the pex_config package has been used since December 2011. It contains features such as selection of an algorithm by name from a registry, automatically pulling in the algorithm's configuration. Tools are provided to print out the history of any parameter.

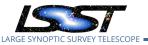
4.5 Logging

The logging service is used by application and middleware code to record status, diagnostic, and debugging information about their execution.

4.5.1 Key Requirements

Log messages must be associated with component names organized hierarchically. Logging levels controlling which messages are produced must be configurable on a per-component

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level. There must be a way for messages that are not produced to not add significant overhead. Logs must be able to be written to local disk files as well as sent via the event subsystem. Metadata about a component's context, such as a description of the CCD being processed, must be able to be attached to a log message.

4.5.2 Baseline Design

Log objects are created in a parent/child hierarchy and associated with dotted-path names; each such Log and name has an importance threshold associated with it. Methods on the Log object are used to record log messages. One such method uses the C++ varargs functionality to avoid the overhead of formatting the message until it has been determined if the importance meets the threshold. Log messages can have additional key/value contextual metadata associated with them through a per-thread diagnostic context.

4.5.3 Implementation

The logging implementation in the log package is based on the Apache log4cxx package [17]. Use of an off-the-shelf package provides the required functionality, including relatively advanced features as thread-safety, with minimal support cost.

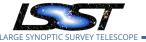
Wrappers were written to adapt the log4cxx classes to LSST needs, providing "syntactic sugar" as well as providing an interface that can be reimplemented in case log4cxx becomes deprecated in the future. The C++ classes and methods were also wrapped with pybind11 to enable compatible access from Python.

log4cxx provides for significant configurability of logs, including their destinations, message formatting, and thresholds, both through code and through external configuration files in either XML or Java property format. An adapter was written to enable log messages to be sent via ActiveMQ events, but this is not currently being used, as log collection mechanisms are adequate.

4.6 MultiNode API

The MultiNode API is used to isolate the applications code from the details of the underlying communications mechanism used to coordinate execution on and transfer data among a

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tightly-synchronized set of nodes.

4.6.1 Key Requirements

The MultiNode API must support at least point-to-point communication, global collection and aggregation of data from a parallel computation with distribution of the aggregate back to parallel processes, and data exchange from processes to "neighboring" processes using a defined geometry. It must be possible to send and receive objects, but transmission of complex data structures involving pointers is not required.

4.6.2 Baseline Design

The MultiNode API will be an abstract interface used by applications code implemented using two technologies: a message broker such as RabbitMQ [13] and MPI [7]. The former will typically be selected for general-purpose, low-volume communication, particularly when global publish/subscribe functionality is desired; the latter will be used for efficient, high-rate communication. A SuperTask will call the MultiNode API with a specification of its desired geometry in order to execute its algorithm in parallel. The algorithm will make explicit use of the MultiNode API to send data to and receive data from other instances of the task, including scatter/gather (or map/reduce) communication.

4.6.3 **Prototype Implementation**

A set of classes have been written that use a batch system and communications via mpi4py [18] to provide a pool of nodes that can be used in map/reduce fashion. Tasks making use of this package subclass the base classes provided by this package and call the API explicitly to map Task and function execution across data distributed over the node pool. This API is used by driver scripts that perform single frame processing, calibration frame processing, coaddition, and multiband measurement.

4.7 MultiCore API

The MultiCore API is used to isolate the applications code from the details of the underlying threading mechanism used to coordinate execution on muliple cores on one node.

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Use of this API will be necessary to take advantage of current and future processors that contain large numbers of cores but limited amounts of memory per core.

This API has not yet been designed. Given contemporary limitations of threading at the Python level, it is anticipated that it will be implemented only at the C++ level and will likely use an existing API such as OpenMP [9].

Workload/Workflow Management 5

The Workload and Workflow Management component provides management of the execution of science payloads ranging from a single pipeline to a series of "campaigns", each consisting of multiple pipelines. Its services are able to handle massively distributed computing, executing jobs when their inputs become available and tracking their status and outputs. They ensure that the data needed for a job is accessible to it and that outputs (including log files, if any) are preserved. They can allocate work across multiple computing environments, in particular between NCSA and the Satellite Computing Facility at CC-IN2P3.

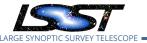
This component invokes SuperTasks (section 4.1) via Activators to sequence the execution of dataflow graphs across one or more distributed computational environments, in particular compute resources allocated via a batch computing service.

5.1 Batch Computing

Batch computing occurs on LSST dedicated computing platforms at NCSA and CC-IN2P3 and potentially on other platforms. Resources other than local CPU and storage for computation, such as curation storage to hold final data products (the Data Backbone, section 2) and network connectivity, are also needed to completely execute a pipeline and completely realize the data handling scheme for input and output datasets; the Workload and Workflow component utilizes these as well.

Computing resources are physical items which are not always fit for use. They have scheduled and unscheduled downtimes and may have scheduled availability. The management of campaigns requires the detection of unscheduled downtimes of resources, recovery of executing pipelines affected by unscheduled downtimes, and arranging for the best use of available resources.

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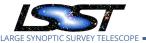


One class of potential resources are opportunistic resources which may be very capacious but may not guarantee that jobs run to completion. These resources may be needed in contingency circumstances. The workload management system is capable of differentiating "kills" from other failures so as to enable use of these resources.

5.2 Workflow Management

The Workflow Management service provides for orchestration and execution of pipelines. Its basic functionality is as follows:

- Pre-job context:
 - Supports pre-handling of any input pipeline data sets when in-job context for input data is not required.
 - Pre-stages input data into a platform's storage system, if available.
 - Produces condensed versions of database tables into portable lightweight format when required.
 - Deals with platform-specific edge services.
 - Handles identities and provides for local identity on the computing platforms.
 - Provides credentials and end-point information for any needed LSST services.
- In-job context:
 - Provides stage-in for any in-job pipeline input data sets.
 - Provides any Butler configurations necessarily provided from in-job context.
 - Invokes the pipeline and collects pipeline output status and other operational data.
 - Provides stage-out for pipeline output data sets when stage-out requires job context.
- Post-job context:
 - Ingests any designated data into database tables.
 - Arranges for any post-job stage out from cluster file systems.
 - Arranges for detailed ingest into custodial data systems.
 - Transmits job status to workload management.



The baseline design for the Workflow Management service uses a workflow tool such as Pegasus [11] together with HTCondor [6], custom Activators, and Data Backbone interface scripts.

5.3 Workload Management

Workload Management considers the ensemble of available compute resources and the ensemble of campaigns to be executed and dispatches pipeline invocations to the Workload orchestration system based on resource availability and campaign priority. It considers pipeline failures reported by the Workload orchestration system, distinguishing errors from computing resources and computational errors where possible, and arranges for incident reports and retrying failed invocations when appropriate. It exposes the progress of each campaign to operations staff and monitoring systems, providing appropriate logging and events.

This service has not yet been prototyped.

6 Processing Control

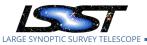
Processing Control provides the highest-level services that manage the execution of scientific payloads within the DMS. There are three main productions that occur on differing cadences:

- Prompt Processing (nightly/daily)
- Template and Calibration Products Production Execution (daily/weekly/annual)
- Data Release Production Execution (annual)

as well as an *ad hoc* OCS-Controlled Batch processing service.

The Production Execution services are primarily managing submissions of campaigns at appropriate times and with appropriate configurations to the Workload and Workflow Management component. Prompt Processing and OCS-Controlled Batch, however, involve custom interaction and control code in order to work closely with the Observatory Control System (OCS).

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6.1 Prompt Processing

The Prompt Processing service retrieves pixel data from the main LSST camera, builds images, and sends them to the Archive Center for processing by the Alert Production payload or the Raw Calibration Validation payload.

The Prompt Processing service is composed of a Data Management Control System (DMCS), a Foreman, and a set of Forwarders at the Base as well as a Foreman, a set of Distributors, and computational worker nodes at NCSA. See Figure 3.

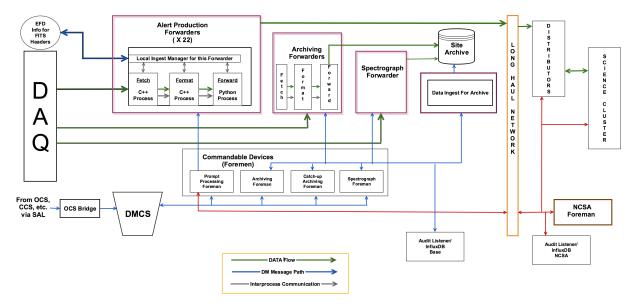


FIGURE 3: Image Ingest and Processing System

The Forwarders at the Base connect directly to the Camera Data System to obtain pixel data, one raft's worth of pixels per forwarder. Fewer forwarders could be used if failures exhaust the available spares. They merge these pixels with header metadata and transfer the resulting images to the NCSA Distributors. The current design uses bbFTP to perform the transfer. The Data Butler clients on the worker nodes pull the received images from the Distributors.

The Foremen at the Base and NCSA track the status of their respective pools of Forwarders and Distributors and reallocate rafts as needed. The NCSA Foreman arranges for the configured science payload to be executed on the worker nodes and collects image quality feedback, transferring it to the Telemetry Gateway service at the base for reporting to the OCS.

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The DMCS is responsible for interfacing with the OCS as a commandable SAL (OCS Software Abstraction Layer) component as defined in LSE-209 and LSE-70. It accepts commands from the OCS to configure, start, and stop prompt processing (as well as several other OCS-related services) and communicates with the Base and NCSA Foremen to do so. Note that the service operates in a data-driven mode; no explicit OCS commands are given to process each image.

This system has been prototyped extensively in the ctrl_iip package and is being used for integration tests with other LSST subsystems.

6.2 OCS-Controlled Batch

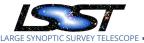
The OCS-Controlled Batch Service provides the ability for OCS scripts to initiate processing at NCSA using data that is already in the Data Backbone with results returned to the Data Backbone and accessible in the usual manner of the project's data. One major use of this is to execute a daily calibration update payload upon completion of the day's calibration image acquisitions.

The OCS-Controlled Batch service works more simply than the Prompt Processing service. The DMCS accepts commands from the OCS that refer to a pre-existing library of available pipelines (SuperTasks). It submits jobs to the Workflow management system at NCSA to execute these on data that resides within the Data Backbone. Job completion and status notifications are returned to the OCS.

This service has not yet been prototyped.

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