Contextual Constraint Modeling in Grid Application Workflows

Greg Graham, Anzar Afaq, David Evans, Gerald Guglielmo, Eric Wicklund
Fermi National Accelerator Laboratory, Batavia, IL, 60510, USA

Peter Love
Department of Physics, Lancaster University, Lancaster, UK

Submitted to
Concurrency and Computation: Practice and Experience
Special Edition for GGF10 Workflows Section
February 1, 2008

Abstract
This paper introduces a new mechanism for specifying constraints in distributed workflows. By introducing constraints in a contextual form, it is shown how different people and groups within collaborative communities can cooperatively constrain workflows. A comparison with existing state-of-the-art workflow systems is made. These ideas are explored in practice with an illustrative example from High Energy Physics.

1 Introduction
The Grid is emerging as a specialized distributed computation standard of unprecedented power and scope, promising to turn commodity networks and computers into commodity computation. The Grid concept has already been proven useful for science in many applications [1][2]. Substantial infrastructure already exists [3] or is being planned [4][5]. Data processing on the Grid ranges from tightly coupled kinds of problems to loosely coupled (the so-called "embarrassingly parallel") ones. Computation involving the use of MPI [6] or some other parallel processing standard within a single application is an example of the former kind. The High Energy Physics (HEP) problem domain is characterized by the latter: parallel independent filtering or data processing applications with large data flows between them. Requirements placed on large processing projects are often coordinated among many interests and groups within a Virtual Organization (VO). In the case of workflows containing a moderate number
of application steps, it becomes a daunting task to check that all of the input parameters and installed software configurations conform to decisions made at the collaboration level. It is useful therefore to have a mechanism with which it is able to specify constraints on the parameters of the individual workflow steps that bring them into line with collaborative decisions coherently across the entire workflow, possibly even dynamically as decisions or discoveries are being made. In the paper, it will be shown that:

- Collections of constraints can be gathered into documents called contexts that function as operators on existing workflow graphs. An algebra of contexts supporting factoring and composition can help different groups within a VO work together through constraint sharing. Decomposition of contexts can allow for variance of constraints simultaneously across several different categories.

- Constraint expressions and contexts form an interesting and hitherto largely unexplored area of data provenance. Knowledge of the constraints implies that it is possible not only to know the values of application input parameters, but also why they were set in particular ways.

It can be assumed that such constraints can be distributed within the stack of a single running application using MPI. However, the techniques developed here find fruitful application in the organizational aspects and in the aspects of sharing collaborative decisions about constraints in the multi-application domain. A partial implementation of these ideas already exists in workflow building tools \[7\] [8] developed for the Compact Muon Solenoid (CMS) \[9\] experiment, a HEP experiment based at the European Center for Nuclear Research (CERN) \[10\] in Geneva, Switzerland.

In the following, we will focus mainly on semantic constraints and not constraints on physical resources, synchronization, nor parallelization. Many traditional workflow specification schemes such as DAGMan \[11\] and constraint languages such as ClassAds \[12\] already address these concerns. In sections \[2\] and \[3\] it will be shown how multigraphs, including new arrow types called metadata flows, can be used to express constraints. It will also be shown how these constraints can be expressed in cooperating context documents. And a general procedure for reducing multigraphs into fully constrained workflow descriptions suitable for execution by a workflow manager such as DAGMan will be outlined. Section \[4\] will illustrate the concepts introduced in previous sections with an illustrative example from High Energy Physics. Finally, the discussion will be wrapped up and comparisons with existing workflow systems will be made in the conclusion.
2 Objects and Operations in a Workflow Constraint Specification

Workflow specifications are often expressed as directed graphs. In many cases where the workflow consists of pure filtering and/or simple single-pass processing, these graphs are directed acyclic graphs (DAGs). Let \( G = (N, A) \) be a general unconstrained workflow graph. Each node \( N \) in \( G \) corresponds to an application and the set of arrows \( A \) corresponds to a partial sequencing of the nodes, usually generated by real data flow relationships\(^1\). Each of these nodes may have attributes specifying input parameters to or conditions on the corresponding application. In order to express constraints on \( G \), one may add both nodes and arrows. The resulting data structure is a multigraph\(^2\). The extra arrows correspond to constraint relationships between specific node attributes. These extra arrows will be called metadata flows, and the set of all metadata flow arrows constraining a graph \( G \) will be denoted by \( F \). In addition to metadata flows, special nodes may be added whose only purpose is to serve as sources or sinks for metadata flows. These extra nodes are called metadata terminals, and the set of these will be denoted \( M \). This is illustrated in figure 1. An example of a metadata source terminal is a null workflow node that holds a query result from some catalog. An example of a metadata sink is a node that may consume metadata merely to record it, such as a tracking system or provenance recorder.

In general, metadata sources and sinks may be replaced by a single source and a single sink node, but we may also allow for many. The multigraph containing \( G \) and its constraints expressed by \( F \) and \( M \) will be denoted \( M_G \). This is the constrained and unreduced workflow graph. Several types of arrows are evident in \( M_G \) including conventional workflow sequencing arrows and metadata flows. For a summary of all of the symbols being introduced, please refer to table 2.

Operations on the unreduced constrained graph consist of reduction operations that satisfy the metadata flows and thereby gradually reduce \( M_G \) to a constrained and reduced \( G' \), or a workflow graph with zero metadata flows. Let \( F(I.i, J) \) denote a metadata flow, where \( I \) is a node in \( N \) and \( J \) is a node in \( N + M \), and \( i \) is an attribute in \( I \). The first argument is the target of the constraint while the second argument is the domain. A reduction \( R_F \) over \( F \) is an operation that replaces the value of attribute \( I.i \) by some value which satisfies the constraint computed from the domain \( J \). For example, the simplest such operation is just the assignment reduction \( =_F \). The constraint \( I.i =_F J.j \) on \( I.i \) is that it be equal to \( J.j \) where \( j \) is some attribute in \( J \).\(^3\) Categorically, the unifying character of this picture can be seen by considering that general constraint reductions targeting an attribute value in some workflow node are

---

\(^1\)Alternatively, the nodes may correspond to data products and the arrows may correspond to data transformations, as in the Chimera Virtual Data System\(^{13}\). These two pictures are equivalent.

\(^2\)A graph comprises some set \( N \) of nodes and a set \( A \) of arrows such that for any two nodes \( N \) and \( M \) in \( N \), \( N \) and \( M \) can have at most one arrow \( a \) in \( A \) between them. In a multigraph, the restriction on the number of arrows is dropped.

\(^3\)Or, more generally, \( j \) can be a simple expression involving attributes of \( J \).
Figure 1: (A) A simple four application acyclic workflow graph. In order to execute the graph, all node attributes must be set. (B) This simple graph is augmented with metadata flows (pink) specifying various constraints on the node attributes. In addition a metadata source node has been added. The constraint augmented workflow is now a multigraph.
Table 1: The above table summarizes the different graph entities introduced in section 2. (Context will be defined in section 3.)

| Graph | name | Nodes | Arrows |
|-------|------|-------|--------|
| $G$   | Workflow Graph | $N$   | $A$    |
| $F$   | Metadata Flows  | -     | $F$    |
| $M$   | Metadata Terminals | $M$ | -      |
| $C$   | Context         | $M$   | $F$    |
| $M_G$ | Constrained Unreduced Workflow | $M + N$ | $A + F$ |
| $M'_G$ | Metadata Flow Subgraph | $M + N$ | $F$ |
| $G'$  | Constrained and Fully Reduced | $N$ | $A$ |

equivalent to constant assignment reductions emanating from a single metadata terminal node [14].

Let $M'_G$ be the metadata flow subgraph of $M_G$ such that $M'_G$ contains all of the nodes of $M_G$ but only the arrows in $F$. It should be noted that this subgraph should be acyclic so that at least one serialization of the metadata flows $F$ exists. Otherwise the constraint model is undefined. Metadata flows may exist to carry metadata to a finite number of graph nodes in a possibly cyclic $G$, and each node in $G$ has a finite number of attributes. Thus it is always possible to find a finite spanning tree if there are no more than one metadata flow per target attribute.

Reduction always results in the removal of a single arrow from $F$ and possibly the alteration of at most one attribute in the target node of the flow. The order of reduction is determined by a partial ordering of the nodes in $M'_G$. Another possibility is to check and raise an exception in case a boolean constraint evaluates to false. Reduction can continue until $M_G$ has been transformed into $G'$. Nonetheless, there are many such reduction partial orders. Some optimization may be gained by grouping some reduction operations together if it is known in advance that they can be reduced together.

3 Constraints and Contexts

It is useful at this point to introduce the context $C$, consisting of the metadata terminals alone and the metadata flows. By partitioning $M_G$ into a context part $C$ and an application workflow part $G$, we gain the possibility that a single set of constraints agreed upon by some large organization can be applied to multiple application workflow graphs, and that a given application workflow graph can be run in a variety of contexts. Furthermore, we gain the possibility of factoring the context $C$ itself into parts that are of interest to specific individuals or groups.

Given the wide variety of workflow graphs and contexts possible, it is a non-trivial task to design an algebra by which these sets can be combined in a simple way. A further problem is that $C$ by itself is not even a well-defined graph because some of the arrows in $C$ point to nodes that are not in $C$. The approach
taken here to deal with these problems is to assign types to the graph nodes in the application workflow graph. By surveying the set of all possible application nodes in an organization, it is possible to come up with a context document $D_C$ that, rather than being a graph subset, is a collection of rules for how to apply metadata terminals and metadata flows in a real application workflow graph as workflow nodes are added into the context document. The rules are indexed by node type and may be applied under one of two kinds of semantics: "only-once" semantics or "for-each" semantics. For metadata terminals, the only-once semantics are generally used. For metadata flows, the for-each semantics are generally used. This is illustrated in figure 2. This approach works for a large number of cases.

An algebra for combining different context documents is being developed. This is somewhat more difficult to do in complete generality not only since the documents are not graphs, but also because rules must be developed to handle metadata collisions when metadata flows share the same target. In general we would like to avoid that the final metadata flow that gets applied depends upon the order in which the context documents are processed. Even in the absence of a full collision resolution algorithm, there is still a large class of problems for which the metadata flows do not collide and are yet useful. There is also another set of problems for which the "shadowing" behavior of overlapping metadata flows is actually desirable, such as for simple replacement of site dependent variables with a site independent default.

![Figure 2: An illustration of a context document. The application workflow node type (added in the center) is used to lookup rules for adding metadata flows and/or metadata terminal nodes. Generally, flows are added with "for-every" semantics and nodes are added with "only-once" semantics.](image-url)
4 Applications

Many of the ideas presented in this paper have been implemented in the area of data processing for HEP. Two related software toolkits have been developed for that application and will be discussed here:

- The RunJob Project at Fermilab [7] provides basic entities to help define, configure, and execute a workflow. RunJob has metadata terminals, metadata flows, a reduction algorithm, and context documents.

- MCRunjob is a package to create Monte Carlo simulation jobs for the CMS [9] experiment. MCRunjob is based upon the software provided by the RunJob Project.

In the following, the problem of offline data processing and analysis in HEP will be described in very broad terms. Then the basic entities provided by the RunJob Project will be described, and a concrete example of the contextual application of constraints will be described.

4.1 High Energy Physics Data Analysis

The expected volume of data from the Large Hadron Collider (LHC) experiments at CERN [4][15] is expected to be very large, on the order of several petabytes of data per year. Distributed processing of this data is expected to be the norm instead of the exception, both because of the data volume and because the collaborators on these experiments are expected to be able to make significant contributions to LHC analysis without traveling to CERN for extended periods of time. New tools and frameworks must be brought to bear to help organize the resources towards the successful processing and analysis of data under these circumstances, and this in fact generates the interest of HEP in Grid technology.

The successful analysis of HEP data involves the production and analysis of large amounts of simulated "Monte Carlo" data also in order to understand detector responses and biases that could affect a measurement. The amount of Monte Carlo data produced will be of the same order of size as the actual data collected. The production of Monte Carlo usually involves a sequence of application programs. The following are just three broad examples.

- Generator program: This program randomly generates a pure physics event taking into account theoretical probabilities for the production of subatomic particles and fast decay products associated with a collision event.

- Simulator program: This program steps each particle created by the generator through a precise model of the collider detector, and calculates the amount of energy deposited in each defined detector volume. An LHC generated event may contain dozens of individual particles to track, but the collider detector may contain hundreds of thousand to millions of individually modeled detector volumes.
• Digitizer program: An "active" detector volume is one which is instrumented in the corresponding real detector. For each active detector volume, this program calculates a digitized electronic signal taking into account what is known at the time about the electronics.

The perennial problem in the area of distributed Monte Carlo production is to constrain the applications so that the data produced at one site is of the same quality as data produced at any other site.

User analysis is generally approached from the standpoint of how to gain individual access to distributed resources and how to move user written analysis software to the job execution site. However, here we are more concerned with the organizational principles of coordinating the processing data across different user jobs. One possible way to think about this problem is as a constraint. Say users belong to more than one physics analysis group. Each application that the user submits may have dozens to hundreds of parameters to set, and the user will not be able in general to set them all by hand. Often, it is the physics group that provides help in setting all of the "expert" parameters. In other words, the physics group provides a context within which the user must analyze data. This is important especially if the user belongs to more than one physics group. These might include the following.

• Detector parameters that only experts know how to set. For example, thresholds on the cells in the electromagnetic calorimeter. These parameters control whether or not an individual detector component will write data into the output stream (i.e.- only if the simulated signal is above threshold)

• Choice of algorithm to use for the reconstruction of a physics object. For example, jet clustering, and parameters such as a cone size for that algorithm. Such parameters are often set by algorithm specialists and maybe not often set by individual users unless they are doing a study.

• Choice of input dataset. Modern data management systems such as the CMS data management system will have the ability to select datasets by a query on the physics metadata. The queries may differ from group to group.

• User written software. This could contain special user parameters or the specification of special libraries.

In many cases, it is important when comparing two different analyses that such parameters as outlined above are known and controlled for. Other site dependent parameters best set by an administrator include the following.

• locating the input data
• correct placement of the output data.
• locating of the experiment application software and libraries
• accessing local batch or Grid resources
• configuring application parameters governing simulation

4.2 The RunJob Project

The RunJob Project was initiated at Fermilab as a common project between the DZero and the CMS experiments to combine their respective tools used in creating jobs for production of Monte Carlo data. The software produced contains the following elements:

• Modular configuration. Workflow elements consist of modular descriptions of application descriptions and dependencies upon other application descriptions.
• Context driven workflow.
• Simple framework model of workflow execution.
• Reduction algorithm for reducing metadata flows.

A simple diagram illustrating RunJob appears in figure 3.

4.2.1 Modular Configuration

Workflow elements in RunJob contain key/value parameters that configure the application at hand. These parameters can be used to run the application at hand directly or to create a job that will run the application later. Workflow elements in RunJob are also given a complementary key/value pair description. This description is much like a Classed [12] in Condor. A given workflow element has dependencies expressed in terms of the descriptions of other workflow elements. This is used to determine execution order of the workflow elements or of the jobs they create if they are making jobs.

Finally, parameters in a workflow element are allowed to be references to parameters in other workflow elements by specifying the description of another workflow element to reference and the parameter within that workflow element to reference.

4.2.2 Context Driven Workflow

In the RunJob software, a context document can be given that expresses simple constraints on the parameters known to the workflow elements. Each block of the context consists of the following information:

• A header consisting of a workflow element description
• A body consisting of a list of directives that can either constrain workflow parameters in individual workflow elements, define references between parameters of two different workflow elements, or redefine existing references between two different workflow elements.
Figure 3: (A) The simplified core class structure of RunJob. Workflow elements consist of dictionaries that describe each application. They in turn have descriptions consisting of key/value pairs and lists of dependencies which reference descriptions of other workflow elements. It can reduce a metadata flow using the GetValue method which references a metadata element in another workflow element by specifying elements from its description dictionary. The workflow elements are constrained by an entity called the Linker, which also issues framework messages to the workflow elements. Each workflow element may have a handler registered to handle the framework message are task. (B) An interaction diagram showing the pattern of framework messages for three workflow elements (assumed to be in dependency order) and three framework messages or tasks. Workflow elements may handle the framework call or not.
The context is loaded into the system prior to any workflow elements. When a workflow element is added to the system, the directives within any context block whose header matches the description of the added workflow element are applied to that workflow element. In the RunJob software the match must be exact in the sense that all key/value elements in the context block header must match the workflow element description. Different context documents may be loaded into the system simultaneously. Currently, the RunJob system does not implement any conflict resolution algorithm on similar context blocks emanating from different documents. Rather, the document specified last wins any conflict.

4.2.3 Framework Model of Workflow

In the RunJob software, the workflow is executed in framework fashion. The user can define a set of framework tasks, each framework task being represented by a string. After all workflow elements have been added to the system, it will issue each framework task in the form of a message to each workflow element. The order of the workflow elements is determined by their dependencies. The workflow elements may or may not respond to specific framework calls depending on how they are defined and configured.

This arrangement is logically equivalent to a DAG in the case that there is one framework task and the nodes are laid out in dependency order. The DAG has the advantage that in the case of a node failure, it may proceed to process independent nodes. A comparison of the methods of executing workflow elements is beyond the scope of this paper. Many other workflow systems do in fact use DAGMan, developed at the University of Wisconsin at Madison, as a workflow execution manager.

4.2.4 Reduction Algorithm

Reduction in RunJob is accomplished by lazy evaluation of metadata flows. The metadata flow is evaluated by inter-workflow element lookup only when the target of the metadata flow is accessed by some other entity or metadata flow. This is accomplished by setting read triggers on the attributes of RunJob workflow elements.

4.3 MCRunjob

MCRunjob is a workflow management system based upon the RunJob software for the CMS experiment. MCRunjob, however, is used for building jobs to produce Monte Carlo data; it does not actually execute the jobs themselves.

---

4 This has been relaxed a bit in practice with wildcards.
5 In cases where there are no dependencies to determine order, then the workflow elements appear in the order in which they were added to the system.
Rather MCRunjob executes the workflow of "configuring the jobs in the execution workflow." This is nonetheless an ideal place to implement the ideas in this paper as they have to do with constraints on workflow configuration. MCRunjob produces workflows for execution on DAGMan/Condor-G or on local batch systems.

The simplified MCRunjob workflow in the example contains the following framework tasks:

- **contactDB**: Contact the CMS Production Control Database
- **configureJob**: Reduce constraints by referencing metadata targets
- **makeJob**: Create and store application jobs into the Linker
- **runJob**: Retrieve and submit stored jobs

There is also an implicit reset framework task which is not shown. If the workflow happens to contain a serialized DAG of user applications, then the jobs are written out in the same serial order and synchronized by some external means.

### 4.4 Practical Example

In this section, we present a simple workflow graph $G$ for the CMS experiment. It is operated upon by a series of context documents $C_1$, $C_2$, and $C_3$ resulting in a final unconstrained workflow graph $M_G$ to be subsequently reduced by the RunJob lazy reduction algorithm.

The example here is based upon a real example from Monte Carlo production for the CMS experiment. It is not, however, an actual real life example. The real life examples contain far too many confounding specializations that are required in order to get actual Monte Carlo production done in the current imperfect but evolving Grid infrastructure. Also, real CMS production does not at this time constrain physics parameters by physics group. Rather, all actual production parameters come from a production control database known as the RefDB [16]. In one case, the syntax for the context block headers has been simplified. Finally, many of the names of workflow elements and parameters have been changed to be more illustrative and less comprised of CMS jargon. The applications described were discussed in section 4.

Consider the unconstrained workflow $G$ defined in section 4.1. In this workflow, a user has chosen to run the generator program CMKIN followed by the simulation program OSCAR as well as the Digitization program. The constraint that the input data of one step be read from the output of the previous step is expressed as a metadata flow. In MCRunjob, the workflow graph is just specifying the steps in the creation of a job, so a special "RunJob" workflow element is added at the end to submit the jobs.

---

6 The details of how this workflow is executed efficiently to create $N$ parallel jobs is unimportant here. But briefly, there is a special group called the "onGroup" of framework calls that is executed $N$ times.
The first context file $C_1$ is shown in section A.2 and defines the calls in the RunJob framework, described in section 4. Calls are added to two predefined groups: "preGroup" which is executed only once, and "onGroup" which is executed as many times as there are jobs to be created.

The second context file $C_2$ is a hypothetical context file written by a physics group. (The corresponding real file used for CMS Monte Carlo production is very long and unenlightening.) It exhibits the for-each and once-only semantics described in section 3. For each added workflow node matching a type declaration in the header of a context block, metadata flows are added and dependencies are added. At the bottom of this context file, two metadata terminal nodes are added once only. The RefDB is a metadata source corresponding to the CMS production control database, and the PhysicsGroupDB is a metadata source corresponding to a hypothetical database that could be set up by a physics group to organize parameters that people in the group should use.

The third context file $C_3$ is a scheduler context file. (The corresponding real file used in CMS contains configurations for many different batch systems.) This context file substitutes a concrete choice of a workflow element, LCG::ResourceBroker, for an abstract choice given in the workflow definition, RunJob.

The context files given in the appendices do not collide on metadata targets because they have been organized on the basis of the node types that they modify. No collision algorithm is needed. When the contexts are combined with the workflow, the final unconstrained workflow $M_G$ results. It is given in section sc:wf:unconstr. As explained in section 4, RunJob reduces the unconstrained workflow into a fully constrained workflow graph (not shown) using a lazy algorithm that triggers the evaluation of a constraint when its target is accessed. RunJob does not implement more general Boolean constraints at this time.

Note that if the user had to specify all of the constraints in the final unconstrained workflow, it would be a very complex task. MCRunjob currently tracks about 150 parameters for CMS Monte Carlo production, mostly coming from the RefDB or describing local site conditions. As the system in CMS gets more complex and involves more applications and users, the number of parameters can only be expected to grow. By splitting the work into different context files, the work can be shared among different roles: A naive user creates the initial unconstrained workflow in section A.1, a developer maintains the framework context file in section A.2, a physics group convener maintains the physics context file in A.3, and an administrator maintains the scheduler context file in section A.4.

5 Conclusion and Relation to Other Work

This paper outlined some considerations for constraint modeling in Grid application workflows. We focused mainly on semantic constraints and not constraints on physical resources or monitoring. We have shown how multigraphs and metadata flows can be used to express constraints, and outlined a general procedure
for reducing multigraphs into fully constrained graph workflow descriptions. Finally, we have shown how to factor out the constraints into contexts that can be maintained separately and recombined later in a collaborative effort to constrain a workflow.

5.1 Related Work

In addition to being used in creating jobs in MCRunjob, contexts have been demonstrated that govern the generation of fully constrained workflows as ordered lists of shell scripts, Condor-G/DAGMan [11], or Chimera Virtual Data Language (VDL) [13] all from the same simple workflow. The mechanism is to use a context to select one or more code generators. DAGMan is a complete workflow manager that has a very general model for specifying workflows, but it relies on the user completely to set up both the DAG and the parameters in the DAG itself. VDL presents a unique view of data processing as a network of data products connected by application induced transformations. While it is possible for different collaborators to work independently on different transformations, there are not really tools for allowing collaborators to independently specify different aspects of the same chain of transformations. The context mechanism presented here emphasizes rather the idea of virtual transformation as opposed to the virtual data.

Work on Context Oriented Programming [17] is being done for mobile computing. Systems are being developed to exchange the actual code that gets run in different locales. The present work is different in that it is effectively exchanging constraints and not actual code, although contexts can be fooled into loading different modules as shown in the example. Also, the definition of "locale" here is generalized to be any category of relevance to the VO: physics group, a personal role, etcetera.

Other workflow engines such as Triana [18] and Webflow [19] emphasize graphical user interfaces and allow the user to visually determine where individual elements are executed. Contexts are more suited to text based input. Since they are not graphs, they are more difficult to visualize.

An interesting related work is GridAnt [20]. The problem space of GridAnt is similar: it tries to tame the application space of the Grid by formulating the workflow as an Ant style Makefile with additional procedural constructs. However, it too does not facilitate collaborative workflow in the same way that contexts do.

5.2 Comparison to Cascading Style Sheets

A fresh perspective on the context mechanism of RunJob may be obtained by considering Cascading Style Sheets (CSS)[21]. A CSS document is loaded into a browser before processing HTML documents. The CSS document consists of blocks with headers designed to match hierarchically defined segments of an HTML document. When an HTML document is loaded, each HTML element is processed according to configuration directives contained within a block of CSS.
corresponding to the segment in which the HTML element appears. A RunJob context is thus like CSS for workflow configuration. Though the context block headers of RunJob don’t appear to be hierarchial, they can be if one chooses an ordered sequence of keys to use in workflow element descriptions.

5.3 Contextual Constraints and Provenance

Provenance deals with the problem of collecting all of the information needed in order to recreate a data product. The transformation graph approach of Chimera is most useful here [13]. Detailed provenance is therefore built into the system. However, the prospect of saving metadata flows and metadata terminal nodes before the process of reduction begins on a constrained workflow graph offers the possibility of saving a new kind of provenance. Namely, in addition to saving the flat values of all of the parameters that go into creating a data product, one can also save the constraints and relationships among those parameters and, by extension, why the parameters in a conventional provenance have the values that they do: which calibration set is being used, is it being used across all workflow steps, who signed off on the set of constraints as a whole and not just considering each constraint one by one. This is because the provenance as expressed in a workflow constraint mechanism is categorical.

A Example Workflow Specification Files

The following sections contain code from CMS MCRunjob. The language is called "macro language". Each statement in macro language is interpreted to specific calls on the RunJob API. In the future, the macro language will be deprecated in favor of using the RunJob API directly and expressing workflows and contexts in pure Python. The statements of the macro language below are generally self explanatory.

A.1 Unconstrained Workflow Definition

This unconstrained workflow creates workflow elements for three CMS applications described in section 4 and links them together. The condition that one application read input from the output of the previous step is expressed as a metadata flow.

attach CMKIN
attach OSCAR
OSCAR adddep CMKIN
OSCAR define inputFile ::CMKIN:outputFile
attach Digitization
Digitization adddep OSCAR
Digitization define inputDataset ::OSCAR:outputDataset
Digitization define inputRunNumber ::OSCAR:outputRunNumber
attach RunJob
A.2 Framework.ctx

The following context file simply defines the content and ordering of the framework calls issued by the Linker. The "preGroup" is executed first exactly once, and the "onGroup" is executed as many times as there are jobs to create.

```plaintext
framework define preGroup contactDB
framework define onGroup configureJob, makeJob, runJob
```

A.3 PhysicsGroup.ctx

The following context file is a hypothetical physics group context. It requires the addition of two metadata sources: the CMS production control database RefDB and a hypothetical physics group database. Parameters for various applications are constrained either directly in the context or are constrained by metadata flows from one or the other database. Special directives are given to ensure that connections are opened when the Linker issues the "connectDB" framework call. The description keys are "Database" for the RefDB and the PhysicsGroupDB, and "Application" for the CMS physics applications.

```plaintext
contextBlock Database=PhysicsGroupDB,RefDB
    oncall contactDB do connectToDatabase
end
contextBlock Application=CMKIN, OSCAR, Digi
    add dependency Database=PhysicsGroupDB
    add dependency Database=RefDB
end
contextBlock Application=CMKIN
    define ApplicationVersion 6.133
    define ApplicationName kine\_make\_ntuple.exe
    define HiggsMass ::PhysicsGroupDB:HMass2004
    define TopMass ::PhysicsGroupDB:TMass2004
end
contextBlock Application=OSCAR
    define ApplicationVersion OSCAR\_3\_6\_5
    define HCal On
    define ECal On
    define ECalThreshold ::PhysicsGroupDB:ECalThreshold2004
end
contextBlock Application=Digitization
    define ApplicationVersion ORCA\_8\_4\_1
    define PileupRate ::RefDB:Lumi_1032
end
attach PhysicsGroupDB
attach RefDB
```
A.4 Scheduler.ctx

The following context file defines the alias "RunJob" to mean "LCG_ResourceBroker". When the novice user adds the generic "RunJob" element to a workflow, he/she gets the LCG_ResourceBroker element when this context is loaded. The context also contains configuration information for the LCG_ResourceBroker. The tag "@args" means that the metadata flow comes from command line arguments.

```plaintext
namespace add RunJob Scheduler=LCG_ResourceBroker
contextBlock Scheduler=LCG_ResourceBroker
define UserJDLFile ::@args:UserJDLFile
define ResourceBroker ::@args:ResourceBroker
oncall RunJob do submit
end
```

A.5 Full unconstrained Workflow Definition

The above context files are loaded into the system first. (Remember that the PhysicsGroup.ctx also adds two metadata sources at this time.) Upon addition of each element from the workflow of section A.1, the metadata flows and other directives from matching context blocks are added to that element. The following final unconstrained workflow appears below. The metadata flows are reduced out as elements are accessed.

```plaintext
framework define preGroup contactDB
framework define onGroup configureJob,makeJob,runJob
attach PhysicsGroupDB
PhysicsGroupDB oncall contactDB do connectToDatabase
attach RefDB
RefDB oncall contactDB do connectToDatabase
attach CMKIN
CMKIN add dependency Class=PhysicsGroupDB
CMKIN namespace add PhysicsGroupDB Class=PhysicsGroupDB
CMKIN add dependency Class=RefDB
CMKIN namespace add RefDB Class=RefDB
CMKIN define ApplicationVersion 6.133
CMKIN define ApplicationName kine\_make\_ntuple.exe
CMKIN define HiggsMass ::PhysicsGroupDB:HMass2004
CMKIN define TopMass ::PhysicsGroupDB:TMass2004
attach OSCAR
OSCAR add dependency Class=PhysicsGroupDB
OSCAR namespace add PhysicsGroupDB Class=PhysicsGroupDB
OSCAR add dependency Class=RefDB
OSCAR namespace add RefDB Class=RefDB
OSCAR define ApplicationVersion OSCAR\_3\_6\_5
OSCAR define HCal On
OSCAR define ECal On
```
OSCAR define ECalThreshold ::PhysicsGroupDB:ECalThreshold2004
OSCAR adddep CMKIN
OSCAR define inputFile ::CMKIN:outputFile
attach Digitization
Digitization add dependency Class=PhysicsGroupDB
Digitization namespace add PhysicsGroupDB Class=PhysicsGroupDB
Digitization add dependency Class=RefDB
Digitization namespace add RefDB Class=RefDB
Digitization define ApplicationVersion ORCA\_8\_4\_1
Digitization define PileupRate ::RefDB:Lumi\_1032
Digitization adddep OSCAR
Digitization define inputDataset ::OSCAR:outputDataset
Digitization define inputRunNumber ::OSCAR:outputRunNumber
attach LCG_ResourceBroker
LCG_ResourceBroker define UserJDLFile ::@args:UserJDLFile
LCG_ResourceBroker define ResourceBroker ::@args:ResourceBroker
LCG_ResourceBroker oncall RunJob do submit
framework run

References

[1] I. Foster and C. Kesselman, ed. The Grid: Blueprint for a New Computing Infrastructure, 2nd Edition, Morgan Kaufmann (2004)

[2] F. Berman, G. Fox, and T. Hey. Grid Computing: Making The Global Infrastructure a Reality, John Wiley & Sons, (2003)

[3] Grid2003 http://www.ivdgl.org/grid2003

[4] Enabling Grids for E-sciencE http://public.eu-egee.org/

[5] Open Science Grid http://www.opensciencegrid.org

[6] Gropp, W. et al. Using MPI: Portable Parallel Programming with the Message-Passing Interface. The MIT Press, Cambridge, Massachusetts, 3rd printing, 1996.

[7] The RunJob Project homepage http://projects.fnal.gov/runjob

[8] G.E. Graham, et al. MCRunjob: A High Energy Physics Workflow Planner for Grid Production Processing Proceedings of CHEP 2003 (TUCT007) San Diego

[9] The CMS Experiment homepage: http://cmsinfo.cern.ch

[10] CERN Laboratory homepage: http://www.cern.ch

[11] DAGMan: http://www.cs.wisc.edu/condor/dagman

18
[12] Raman, R. and Livny, M. "Matchmaking: Distributed Resource Management for High Throughput Computing" Proceedings of the Seventh IEEE International Symposium on High Performance Distributed Computing, July 28-31, 1998, Chicago, IL.

[13] I. Foster, et al. "Chimera: A Virtual Data System for Representing, Querying, and Automating Data Derivation" 14th International Conference on Scientific and Statistical Database Management (SSDBM 2002)

[14] B. Pierce. Basic Category Theory for Computer Scientists. MIT Press (1991)

[15] The ATLAS Experiment homepage: [http://atlas.web.cern.ch/Atlas/](http://atlas.web.cern.ch/Atlas/)

[16] CMS Internal Note 2002/044 [http://cmsdoc.cern.ch/cms/production/www/documents/RefDB/in02_044.ps](http://cmsdoc.cern.ch/cms/production/www/documents/RefDB/in02_044.ps)

[17] R. Keays. Context Oriented Programming. PhD Thesis, University of Queensland, Australia (2002)

[18] "Triana Workflow" [http://www.triana.co.uk](http://www.triana.co.uk)

[19] Bhatia, D. et al. "WebFlow - A Visual Programming Environment for Web/Java Based Coarse Grain Distributed Computing." Concurrency: Practice and Experience, vol. 9, no. 6, p. 555 (1997)

[20] von Laszewski, G. et al. "GridAnt: A Client-Controllable Grid Workflow System" 37th Hawaii International Conference on Computer Science, Hawaii, USA (2004)

[21] Cascading Style Sheets [http://www.w3.org/Style/CSS/](http://www.w3.org/Style/CSS/)