A Scientific Workflow Model Designer based on Scientific Information Control Nets

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***Abstract*—In this paper, we design and implement a scientific workflow process designer with a conceptual building block depicting its architectural structure. The designer is theoretically designed from the scientific information control net[1], and it is graphically implemented by expanding the standardized BPMN(business process modeling notations)[2]. In particular, the designer is able to automatically transform a BPMN-based graphical form into an XML-based textual form of the scientific workflow process model. Finally, we illustrate two captured-screens of the designer, as an operational example, which are corresponding to a simple scientific workflow process model and its XML-based representation, respectively.**

***Keywords*-scientific workflow; information control net; data intensive workflow; formal workflow description; scientific workflow model designer**

I. Introduction

Traditionally, the goal of a workflow management system was to describe, control, and monitor the enactments of business procedures in a workflow-supported organization. According to flourish on the almost all industries through the various types of process-driven business models, such as process portals, POD (Process-on-Demand), process choreography and orchestration, process collaboration, and inter-organizational workflows, the applicability of the workflow management system has been changing, broadening, and scaling up, too, along with dramatic progressions of workflow and business process technologies. In recent, what we see happening now in the workflow literature is that the applicability reaches up to the scientific knowledge discovery arena, which is so-called "Scientific Workflow[3][4]," that is able to not only support the whole stage of scientific experiments and simulations but also automate exploratory processes for discovering scientific knowledge involving cycles of observation, hypothesis formation, experiment design and execution. At this point, we would faithfully follow the conceptual definition of the scientific workflow stated in [3],[4], and [5], the like of which the scientific workflow implies the large scale and data intensive workflow, in terms of describing and deploying the overall idea and the basic concepts throughout the paper.

In this paper, we particularly focus on the quality of service issues in scientific workflow technologies, in terms of efficient load-balancing strategies in designing a large scale scientific workflow enactment architecture, and effective exception handling and recovery strategies in implementing a data intensive scientific workflow system. In order to cope with these quality of service issues, we need a well-defined scientific workflow meta-model that is surely applicable to the scientific workflow model as well as the architectural functionality of the underlying scientific workflow system. As we know, there exist tens of proposals[6][7][8][9] and rationales[5][10] about defining the concept of scientific workflow models and systems, so far. However, we, in this paper, try to newly define a scientific workflow meta-model rather than choosing one of those existing scientific workflow models. We also extend the conventional information control net methodology[11] to graphically and formally represent the scientific workflow model spawned from the defined meta-model, which is dubbed "Scientific Information Control Net" that is abbreviated to **sclCN**, from now on.

In organizing the paper, we start from defining the basic concept of the scientific workflow meta-model with a series of functional definitions of the scientific activity types. The next section formalizes the scientific information control net and applies its graphical and formal representation to a pseudo scientific workflow model with describing the implications of the proposed mathematical formalism for large scale and data intensive scientific workflows. And next section describes the structure of the proposed scientific workflow designer. With describing an implementation of nodes which is support a scientific workflow model that is the information contol nets, we finalize the paper.

II. Scientific Workflow Model

In this section, we define a scientific workflow meta-model for modeling scientific experimental processes characterized by the large scale and data intensive properties. Based upon the meta-model, we are able to instantiate sclCN-based scientific workflow models that are conceptually extended from the information control net methodology[11][12].

A. Meta-Model

In order to clearly define a scientific workflow model, it is needed to design a meta-model that is used to be signified by a set of entity types and their relationships. Furthermore, we have to take account of the conceptual definition of scientific workflows to conceive a reasonable and applicable meta-model. In general, the scientific workflow model is

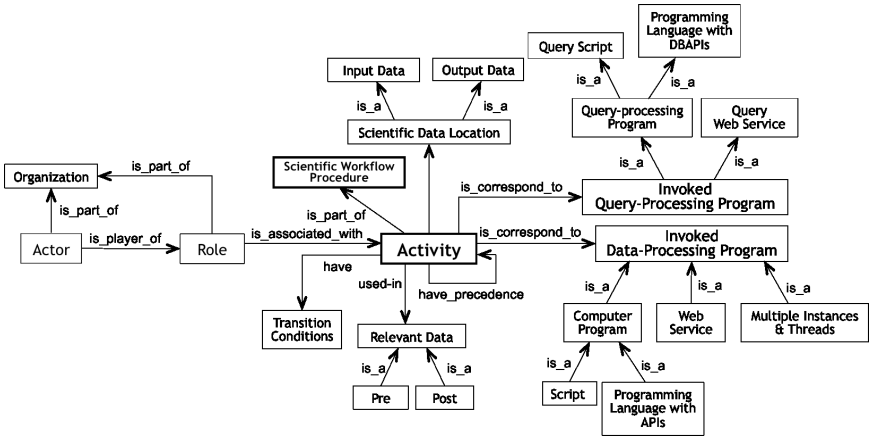

Fig. 1. Meta-model for Modeling Scientific Workflows

a mathematical methodology to specify various phases of the large and complex science process involving cycles of modeling and automation of computational experiments, data analysis, and data management. The well-described conceptual definition of the scientific workflows was introduced in the project DAKS[5] as followings:

"*A scientific workflow is the description of a process for accomplishing a scientific objective, usually expressed in terms of tasks and their dependencies. Typically, scientific workflow tasks are computational steps for scientific simulations or data analysis steps. Common elements or stages in scientific workflows are acquisition, integration, reduction, visualization, and publication (e.g., in a shared database) of scientific data. The tasks of a scientific workflow are organized (at design time) and orchestrated (at runtime) according to data-flow and possibly other dependencies as specified by the workflow designer. Workflows can be designed visually, e.g., using block diagrams, or textually using a domain-specific language.*"

We design a scientific workflow meta-model by faithfully reflecting the above definition as much as possible. Figure 1 depicts the scientific workflow meta-model drawn from in-depth discussions in the authors' collaborative research groups. The primitive entity types constituting the scientific workflow model are Activity and Tasks (Invoked Query-processing program and Invoked Data-processing program) entity types; the primitive entity types has also certain associations with their own supplementary entity types, like Role, Data Location, and Relevant Data. The followings are the basic definitions of the primitive entity types:

- An **Activity** is a conceptual entity of the basic unit of work (computational task or step), and the activities in a scientific workflow model have precedence relationships, each other, according to their execution sequences based upon data-flow dependencies and/or a temporal ordering of computational steps. Also, the activity entity can be precisely specified by one of the elementary entity types, G-type, D-type, Q-type, and DQ-type, as depicted in Figure 2.
  - The elementary activity implies a computational step that can be realized by either data-processing (D-type), query-processing (Q-type), or both (DQ-type) applications implemented through computer programs, threads, transactions, query-scripts, or web services. Especially, we suppose that the D-type and Q-type activities can be realized by applying the concepts of multiple instance patterns[5], like Multiple Instances with a Priori Design Time Knowledge and Multiple Instances with a Priori Run Time Knowledge implemented in Kepler[7][13]. Also, the D-type data processing activity implies a kind of computational steps for scientific simulations or data analysis tasks performing acquisition, integration, reduction, visualization, or publication (e.g., in a shared database) of scientific data.
  - Particularly, the gateway (G-type) activity means a pair of split-join pseudo step that is used to controlling execution sequences of elementary/compound computational steps. Also, we assume that each of the gateway steps forms in the structured properties, *matched pair* and *proper nesting*. There are three sorts of G-type activities, such as conjunctive gateway (paralleling), disjunctive gateway (alternating), and iterative (looping) gateway. Particularly, the disjunctive gateway needs to be set some specific **Transition Conditions** in order to select one of the possible transition paths during the execution time. The transition condition itself can be defined by using certain input/output relevant data registered on the **Relevant Data** repository.
  - Additionally, there may be a special computational step, the compound activity, that signifies a computational step containing another scientific workflow model, which is so-called **Subprocess**.
- A **Scientific Workflow Procedure** is defined by a predefined or intended set of tasks or computational steps, called Activities, which reflects the activities' temporal ordering of executions and/or data-flow dependencies. A system, so-called scientific workflow management system, helps to organize, control, execute,and monitor such defined scientific workflow models. Conclusively, a

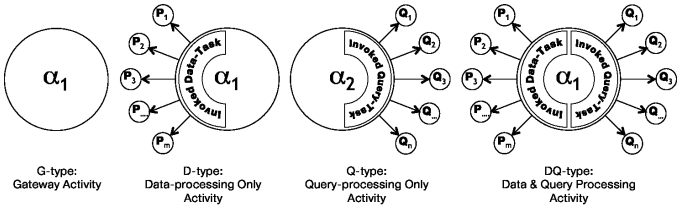

Fig. 2. Activity Types of Scientific Workflows

scientific workflow model can be described by a temporal order of the associated computational steps through the combinations of sequential logics, conjunctive logics (after activity A, do activities B and C, simultaneously), disjunctive logics (after activity A, do either activity B or C, alternatively), and iterative logics, as illustrated in Figure 3.

B. Scientific Information Control Net

In this paper, we would extensively adopt the original information control net (ICN) methodology[11] as the scientific workflow modeling methodology, which is dubbed to sclCN-based scientific workflow model upon the meta-model described in the previous subsection. Based upon the scientific information control net, we are going to dig up a possible way of analyzing activity dominancies on a scientific workflow model in the next section. The scientific workflow model needs to be described by a formal representation so that it is able to provide a means to eventually specify the model either in textual language or in database format, or in both. The following definition is the formal representation of the scientific information control net:

Definition 1: sclCN: **Scientific Information Control Net** of the scientific workflow model. A basic sclCN is 10-tuple $\Gamma = (\delta, \gamma, \lambda, \theta, \varepsilon, \pi, \vartheta, \kappa, \mathbf{I}, \mathbf{O})$ over a set $\mathbf{A}$ of activities (including a set of compound/elementary/gateway computational steps), a set $\mathbf{T}$ of transition conditions, a set $\mathbf{R}$ of relevant data, a set $\mathbf{D}$ of invoked data-task applications, a set $\mathbf{Q}$ of invoked query-task applications, a set $\mathbf{P}$ of scientific roles, a set $\mathbf{L}$ of scientific data locations, and a set $\mathbf{C}$ of participants, where $\wp()$ is the Power-set function.

- $\mathbf{I}$ is a finite set of initial input data locations, assumed to be loaded with information by some external sclCNs before execution of the corresponding sclCN;
- $\mathbf{O}$ is a finite set of final output data locations, perhaps containing information used by some external sclCNs after execution of the corresponding sclCN;
- $\delta = \delta_i \cup \delta_o$
  where, $\delta_o : \mathbf{A} \longrightarrow \wp(\mathbf{A})$ is a multi-valued mapping function of a computational step to its set of (immediate) successors,
  and $\delta_i : \mathbf{A} \longrightarrow \wp(\mathbf{A})$ is a multi-valued mapping function of a computational step to its set of (immediate) predecessors;
- $\gamma = \gamma_i \cup \gamma_o$
  where $\gamma_o : \mathbf{L} \longrightarrow \wp(\mathbf{A})$ is a multi-valued mapping function of a computational step to its set of output data locations,
  and $\gamma_i : \mathbf{L} \longrightarrow \wp(\mathbf{A})$ is a multi-valued mapping function of a computational step to its set of input data locations;
- $\lambda = \lambda_a \cup \lambda_p$
  where $\lambda_p : \mathbf{D} \longrightarrow \wp(\mathbf{A})$ is a single-valued mapping function of a computational step to its invoked data-task application with multiple threads,
  and $\lambda_a : \mathbf{A} \longrightarrow \wp(\mathbf{D})$ is a multi-valued mapping function of an invoked data-task application with multiple threads to its set of associated computational steps;
- $\theta = \theta_a \cup \theta_p$
  where $\theta_p : \mathbf{Q} \longrightarrow \wp(\mathbf{A})$ is a single-valued mapping function of a computational step to its invoked query-task application with multiple threads,
  and $\theta_a : \mathbf{A} \longrightarrow \wp(\mathbf{Q})$ is a multi-valued mapping function of an invoked query-task application with multiple threads to its set of associated computational steps;
- $\varepsilon = \varepsilon_a \cup \varepsilon_p$
  where $\varepsilon_p : \mathbf{P} \longrightarrow \wp(\mathbf{A})$ is a single-valued mapping function of a computational step to one of the scientific roles,
  and $\varepsilon_a : \mathbf{A} \longrightarrow \wp(\mathbf{P})$ is a multi-valued mapping function of a scientific role to its sets of associated computational steps;
- $\pi = \pi_p \cup \pi_c$
  where, $\pi_c : \mathbf{C} \longrightarrow \wp(\mathbf{P})$ is a multi-valued mapping function of a scientific role to its set of associated scientists,
  and $\pi_p : \mathbf{P} \longrightarrow \wp(\mathbf{C})$ is a multi-valued mapping function of a scientist to its sets of associated scientific roles;
- $\vartheta = \vartheta_i \cup \vartheta_o$
  where $\vartheta_o : \mathbf{R} \longrightarrow \wp(\mathbf{A})$ is a multi-valued mapping function of a computational step to its set of output relevant data,
  and $\vartheta_i : \mathbf{R} \longrightarrow \wp(\mathbf{A})$ is a multi-valued mapping function of a computational step to its set of input relevant data;
- $\kappa = \kappa_i \cup \kappa_o$
  where $\kappa_i(\alpha)$: sets of control-transition conditions, $\mathbf{T}$, on each arc, $(\delta_i(\alpha), \alpha), \alpha \in \mathbf{A}$;
  and $\kappa_o(\alpha)$: sets of control-transition conditions, $\mathbf{T}$, on each arc, $(\alpha, \delta_o(\alpha)), \alpha \in \mathbf{A}$;
  where the set $\mathbf{T} = \{default, or(conditions), and(conditions)\}$.

In terms of the graphical representation, we principally adopt the original notations of information control net[11][12]. As depicted in Figure 3, there are possible primitive computation-flows and their related gateway G-type activities. That is, the conjunctive (or parallel) computation-flow type with a pair of conjunctive gateway G-type activities, split-AND and join-AND, is represented by solid dots(•), mean-

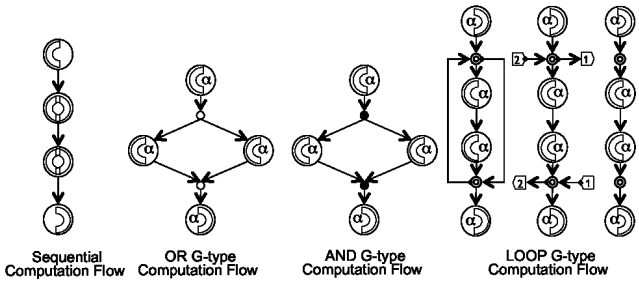

Fig. 3. Logics of Temporal Orders with Gateway Activities in Scientific Workflows

while the disjunctive (or decision) computation-flow type with a pair of disjunctive gateway G-type activities, split-OR and join-OR, is represented by hollow dots(○). Also, the iterative (loop) computation-flow type with a pair of loop gateway G-type activities, split-LOOP and join-LOOP, is represented by double hollow dots.

Besides, in order to be syntactically safe, it is very important for these gateway G-type activities to keep the structured properties—proper nesting and matched pair properties. Therefore, in specifying a scientific information control net, not only each of the gateway G-type activities always keeps matched pair with split and join types, but also multiple sets of the gateway G-type activities keep in a properly nested pattern.

III. Scientific Workflow Model Designer

In order to define a scientific workflow model, it is needed to implement a designer that is a scientific workflow model designer supporting scICN. So, we have implemented a scientific workflow model designer.

The proposed scientific workflow designer is based on standard workflow model designer which support plug-in extension. As fallow workflow/BPM standard that is BPMN, it is easy integrate and execute a workflow/BPM engine like Activiti[14] which is an open source software.

In scICN designer, nodes are able to define three type activities, Q-Type, D-Type and DQ-Type, use an extensible function for workflow standard modeling notation that is the BPMN[2]. But, it could not define 'G-Type' activity, instead as it is 'Gateway' nodes of BPMN. That gateway nodes could describe the conjunctive or parallel logic of scientific workflow model.

And, this designer should be generate executable language for execution of the defined scientific workflow model, executable language would be an extension of BPMN and BPEL.

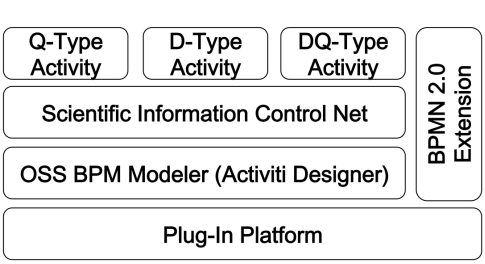

Fig. 6. The Conceptual Building Block of the Scientific Workflow Model Designer

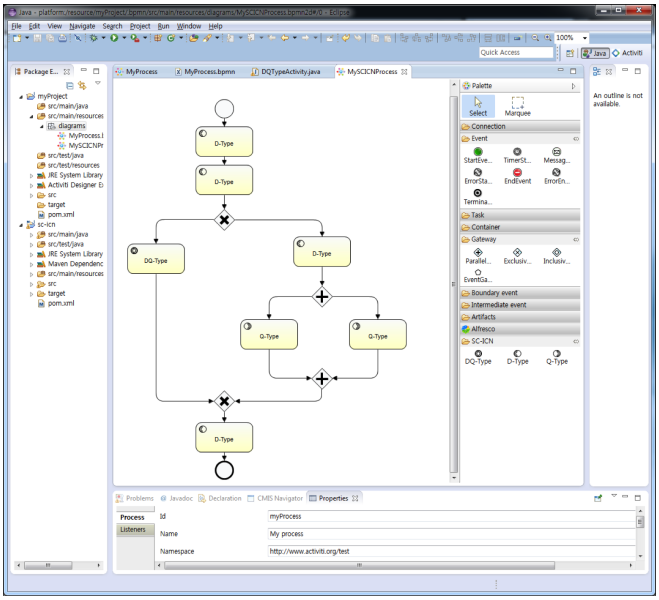

Fig. 4. The scICN Scientific Workflow Model Designer

```
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 xmlns:activiti="http://activiti.org/bpmn" xmlns:bpmndi="http://www.omg.org/spec/BPMN/20100524/DI"
 xmlns:omgdc="http://www.omg.org/spec/DD/20100524/DC" xmlns:omgdi="http://www.omg.org/spec/DD/20100524/DI"
 typeLanguage="http://www.w3.org/2001/XMLSchema" expressionLanguage="http://www.w3.org/1999/XPath"
 targetNamespace="http://www.activiti.org/test">
  <process id="myProcess" name="My process" isExecutable="true">
    <startEvent id="startevent1" name="Start"/>
    <endEvent id="endevent1" name="End"/>
    <serviceTask id="servicetask1" name="D-Type" activiti:class="ctrl.sc_icn.runtime.DTypeJavaDelegation"
    activiti:extensionId="ctrl.sc_icn.servicetasks.DTypeActivity"/>
    <serviceTask id="servicetask2" name="D-Type" activiti:class="ctrl.sc_icn.runtime.DTypeJavaDelegation"
    activiti:extensionId="ctrl.sc_icn.servicetasks.DTypeActivity"/>
    <exclusiveGateway id="exclusivegateway1" name="Exclusive Gateway"/>
    <serviceTask id="servicetask3" name="DQ-Type" activiti:class="ctrl.sc_icn.runtime.DQTypeJavaDelegation"
    activiti:extensionId="ctrl.sc_icn.servicetasks.DQTypeActivity"/>
    <serviceTask id="servicetask4" name="D-Type" activiti:class="ctrl.sc_icn.runtime.DTypeJavaDelegation"
    activiti:extensionId="ctrl.sc_icn.servicetasks.DTypeActivity"/>
    <parallelGateway id="parallelgateway1" name="Parallel Gateway"/>
    <serviceTask id="servicetask5" name="Q-Type" activiti:class="ctrl.sc_icn.runtime.QTypeJavaDelegation"
    activiti:extensionId="ctrl.sc_icn.servicetasks.QTypeActivity"/>
    <serviceTask id="servicetask6" name="Q-Type" activiti:class="ctrl.sc_icn.runtime.QTypeJavaDelegation"
    activiti:extensionId="ctrl.sc_icn.servicetasks.QTypeActivity"/>
    <parallelGateway id="parallelgateway2" name="Parallel Gateway"/>
    <serviceTask id="servicetask7" name="D-Type" activiti:class="ctrl.sc_icn.runtime.DTypeJavaDelegation"
    activiti:extensionId="ctrl.sc_icn.servicetasks.DTypeActivity"/>
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    <sequenceFlow id="flow1" sourceRef="startevent1" targetRef="servicetask1"/>
    <sequenceFlow id="flow2" sourceRef="servicetask1" targetRef="servicetask2"/>
    <sequenceFlow id="flow3" sourceRef="servicetask2" targetRef="exclusivegateway1"/>
    <sequenceFlow id="flow4" sourceRef="exclusivegateway1" targetRef="servicetask3"/>
    <sequenceFlow id="flow5" sourceRef="exclusivegateway1" targetRef="servicetask4"/>
    <sequenceFlow id="flow6" sourceRef="servicetask4" targetRef="parallelgateway1"/>
    <sequenceFlow id="flow7" sourceRef="parallelgateway1" targetRef="servicetask5"/>
    <sequenceFlow id="flow8" sourceRef="parallelgateway1" targetRef="servicetask6"/>
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    <sequenceFlow id="flow11" sourceRef="parallelgateway2" targetRef="exclusivegateway2"/>
    <sequenceFlow id="flow12" sourceRef="servicetask3" targetRef="exclusivegateway2"/>
    <sequenceFlow id="flow13" sourceRef="exclusivegateway2" targetRef="servicetask7"/>
    <sequenceFlow id="flow14" sourceRef="servicetask7" targetRef="endevent1"/>
  </process>
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Fig. 5. The Executable Language for scICN Scientific Workflow

IV. Conclusions

So far, this paper has implemented a scientific workflow model designer with expatiation with the formal scientific information control net and its related definitions by extending the original information control net methodology. Based upon these formal and graphical definitions, we are able to construct a scientific workflow model. In recent, the literature needs various, advanced, and specialized scientific workflow modeling methodologies that are well-suitable to the domain of data intensive and very large scale scientific computing environments. We so strongly believe that this work might be one of those impeccable attempts and pioneering contributions for improving and advancing the large scale and data intensive and scientific workflow management technology.

Acknowledgements

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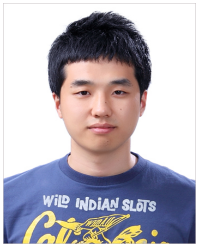

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