

# Workflow Analysis with Quantitative and Structural Metrics

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## Abstract

As scientific workflows grow in complexity and importance, the designers of scientific workflows need a deeper and broader understanding of the characteristics and features of workflows and how they behave in order to improve the overall performance. This paper provides a quantitative, structural and overhead aware analysis of workflows of diverse scientific applications, including astronomy, bioinformatics, earthquake science, and gravitational-wave physics. The workflow analysis is based on novel workflow structural metrics that provide substantial information about the characteristics of workflow structures and concretely show how they influence the overall performance. This paper further applies these metrics to three popular workflow research scenarios including workflow profiling, task clustering and overhead aware task scheduling. Trace based analysis and simulations show their strong capabilities in revealing hidden information and driving improvements on workflow performance.

**Keywords:** Scientific workflows, Performance analysis, Scheduling, Workflow Simulation

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## 1. Introduction

Many computational scientists develop and use complex, data-intensive simulations and analyses [1] that are often structured as scientific workflows, which consist of many computational tasks with complex data dependencies between them. Scientific workflows continue to gain their popularity among many science disciplines, including physics [2], astronomy [3], biology [4, 5], chemistry [6], earthquake science [7] and many more. As scientific workflows grow in complexity and importance, the designers of scientific workflows need a deeper and broader understanding of the characteristics and features of workflows and how they behave in order to drive improvements in algorithms for provisioning resources, scheduling computational jobs, and managing data. Research [8, 9, 10, 11, 12, 13, 14, 15, 16] has been conducted to elaborate the characterization of a wide variety of scientific workflows. In characterizing the execution profile for each workflow, Juve [8] and Callaghan [11] have recently present such metrics as the number of jobs of each type and the I/O, memory, and CPU requirements of each job type from diverse application domains such as astronomy, biology, gravitational physics and earthquake science. Tolosana [10] has proposed 18 metrics to characterize workflow resilience from the perspectives of user, workflow enactor and resource manager. Stampede [12] captures application level logs and resource information, normalizes these to

standard representations, and stores these logs in a centralized general purpose schema.

However, there are still challenges that are not yet solved.

First of all, many of these workflow analysis tools use non-quantitative tools. By quantitative, we first mean the metrics are numerical. Yildiz [13] discussed the appropriateness of standard modeling notations to scientific workflow modeling and present the basic scientific workflow structures. Garijo [17] further introduced detection of common scientific workflow fragments using templates and execution provenance. However, these workflow structures themselves cannot serve as a criterion to evaluate the specific performance of a workflow since they are not numerical. Second, we mean these metrics must be comparable across different platforms and workflows. For example, the average task runtime [8] and the average task failure rate [11] are highly related to the characteristics of execution platforms (system load and resource availability etc.) and thus they do not serve as a reliable metric to guide the design of new optimization methods or a new workflow management system.

Next, there is a lack of utilizing structural information in these workflow analysis tools. Scientific workflows are typically a graph constructed by data dependencies between computational tasks. A data dependency means there is a data transfer between two tasks (output data for one and input data for the other). Data dependencies between workflow tasks play an important role particularly with the emergence of data intensive workflows [11]. Existing metrics [8, 11, 15] (average failure rate, average task runtime, and average resource requirement etc.) treat workflows as no difference to workloads that have no data dependencies between them. Tolosana [10] has touched some basic structural information such as the average number of joins in a workflow. But such metrics cannot tell us a

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global picture of workflow graph such as whether this workflow is dense or sparse, whether this workflow is more sensitive to one particular part of it and whether this workflow is relatively parallel or sequential.

Furthermore, most of these metrics ignore or underestimate the influence of system overheads that play a significant role in the workflow’s runtime [18, 19, 20]. In heterogeneous distributed systems, workflows may experience different types of overheads, which are defined as the time of performing miscellaneous work other than executing users computational activities. Since the causes of overheads differ, the overheads have diverse distributions and behaviors. For example, the time to run a post-script that checks the return status of a computation is usually a constant. However, queue delays incurred while tasks are waiting in a batch scheduling systems can vary widely. In our work, we add overhead as a constitution of the extended workflow graph and this approach allows to apply graph manipulations and graph-theoretic algorithms to the corresponding workflow graphs.

Finally, the community has lacked a deep understanding of these data and how they are related to the overall performance improvement of workflows. In this paper, we propose a series of quantitative and structural metrics that are able to reflect the structure of workflow graphs. Generally speaking, we believe such metrics can (i) guide the formulation of a workflow from the perspective of designers and (ii) help workflow management systems (WMS) refine their orchestration for workflow execution (task clustering and task scheduling etc.). Specifically, in this paper we analyze three usage scenarios including workflow profiling, task clustering, and task scheduling that our metrics can be applied to as discussed below. The reason why we choose these representative areas is related to general picture of how we address issues of performance optimization in scientific workflows. The most straightforward approach is to invest in hardware upgrade and reduce runtime, I/O latency or network latency; for example, replacing current virtual instances with ones that have more CPU, memory or storage resources [21, 22]. However, this approach results in higher IT expenses. Another solution includes varied makespan-centric, DAG scheduling algorithms and heuristics [23, 24, 25] that have been proposed and analyzed. However, these algorithms narrow themselves to the runtime of computational or data transfer jobs. While scheduling remains an NP-hard problem, structural and overhead aware solutions can give new insight to solutions that have not been previously considered. Task clustering [26, 27], job throttling [28], pre-staging [29] and many other solutions have been proposed to reduce the impact of overheads without requiring runtime improvement of computational jobs. In this paper, we not only focus on profiling major overheads occurring in the workflow management systems and revealing their structural connections, but also propose optimization oriented metrics to improve the performance of task scheduling and task clustering.

**Workflow Profiling** is an effective dynamic analysis approach to investigate complex applications in practice. The realistic characteristics of data-intensive workflows are critical to optimal workflow orchestration and profiling is an ef-

fective approach to investigate the behaviors of such complex applications. Traditionally, the common and straightforward approach to address issues of performance optimization is using makespan-centric, DAG scheduling algorithms [30]. While scheduling remains an NP-hard problem, overhead analysis tools can take an important role in giving new insight to solutions that have not been previously considered and that can be further understood. Task clustering [31], job throttling [28], pre-staging [29] and many other solutions have been proposed to reduce the impact of overheads through overlapping overheads and runtimes without requiring runtime improvement of computational jobs. Instead of giving the average task runtime, in Section 4, we propose four metrics to reflect the projection of cumulative overheads on timeline and show how they are related to the overall performance of different workflow optimization methods.

**Task clustering** techniques [20, 31, 32, 27] have been developed to group fine-grained tasks into coarse-grained tasks so that the number of computational activities is reduced and their computational granularity is increased thereby reducing the system overheads. Grouping tasks without considering these dependencies may lead to data locality problems where output data produced by parent tasks are poorly distributed [26]. Particularly, there is a tradeoff between runtime and data dependency balancing and thus a quantitative measurement of workflow characteristics is required to serve as a criterion to select and balance these solutions. To achieve this goal, in Session 5, we propose a series of metrics based on the concept of impact factor and dependency distance that reflect the internal structure (in terms of both runtime and dependency) of the workflow and use these metrics to guide the task clustering during the runtime.

**Task scheduling** [30, 33, 34] has long ignored or underestimate the influence of system overheads. When executing these applications on a multi-machine distributed environment, such as the Grid or the Cloud, significant system overheads may exist [18, 19, 24, 35, 36] and the problem of choosing robust schedules becomes more and more important. Traditionally, a carefully crafted schedule is based on deterministic or statistic estimates for the execution time of computational activities that compose a workflow. However, in such an environment, this approach may prove to be grossly inefficient [36], as a result of various unpredictable overheads that may occur at runtime. Thus, to mitigate the impact of uncertain overheads, it is necessary to choose a schedule that guarantees overhead robustness, that is, a schedule that is affected as little as possible by various overhead changes. In Session 6, we propose a series of structural metrics to evaluate the sensitivity of workflow performance over the overheads and further use them to guide the selection of different scheduling heuristics.

Together, we provide a broader overview of workflow characteristics along with the structural, quantitative and overhead aware metrics. These characterizations can be widely used by the research community to develop synthetic workflows, benchmarks, and simulations for evaluating workflow management systems.

The next Section gives an overview of the related work,

Section 3 presents our workflow and execution environment models, Section 6.2 details our heuristics and algorithms, Section 5.3 reports experiments and results, and the paper closes with a discussion and conclusions.

## 2. Related Work

Some work in the literature has attempted to define and model robustness with metrics. In [37], the authors propose a general method to define a metric for robustness. First, a performance metric is chosen. In our case, this performance metric is the overall runtime including overhead duration as we want the execution time of an application to be as stable as possible. Second, one has to identify the parameters that make the performance metric uncertain. In our case, it is the duration of the individual overheads. Third, one needs to find how a modification of these parameters changes the value of the performance metric. In our case, the answer is, as an increase of the overhead generally implies an increase of the overall runtime. A schedule  $A$  is said to be more robust than another schedule  $B$  if the variation for  $A$  is larger than that for  $B$ . Following this approach, Canon [38] analyzed the robustness of 20 static DAG scheduling heuristics using a metric for robustness the standard deviation of the makespan over a large number of measurement. Braun et al. [25] evaluated 11 heuristics examined and for the cases studied there, the relatively simple Min-min heuristic performs well in comparison to the other techniques.

A plethora of studies on task scheduling [39, 24, 35, 33] have been developed in the distributed and parallel computing domains. Many of these schedulers have been extended to consider both the computational cost and communication cost. A static or statistic estimation of communication cost or data transfer delay [24, 35] has been considered in the scheduling problem. In contrast, we focus on the scheduling overheads that have been ignored or underestimated for long and we demonstrate how their unique timeline patterns influence the overhead robustness.

Workflow patterns [40, 8, 41] are used to capture and abstract the common structure within a workflow and they give insights on designing new workflows and optimization methods. Yu [40] proposed a taxonomy that characterizes and classifies various approaches for building and executing workflows on Grids. They also provided a survey of several representative Grid workflow systems developed by various projects worldwide to demonstrate the comprehensiveness of the taxonomy. Juve [8] provided a characterization of workflow from 6 scientific applications and obtained task-level performance metrics (I/O, CPU and memory consumption). They also presented an execution profile for each workflow running at a typical scale and managed by the Pegasus workflow management system [42]. Liu [41] proposed a novel pattern based time-series forecasting strategy which utilizes a periodical sampling plan to build representative duration series. Compared to them, we discover a common pattern of intervals existing in system overheads while executing scientific workflows. We also leverage this knowledge to evaluate the overhead robustness of existing heuristics and develop new heuristics.

Overhead analysis [19, 18] is a topic of great interest in the grid community. Stratan [43] evaluates workflow engines including DAGMan/Condor and Karajan/Globus in a real-world grid environment. Sonmez [44] investigated the prediction of the queue delay in grids and assessed the performance and benefit of predicting queue delays based on traces gathered from various resource and production grid environments. Prodan [19] offers a grid workflow overhead classification and a systematic measurement of overheads. Our work further investigated the major overheads and their relationship with different optimization techniques. In this paper, we also leverage these knowledge to enhance the existing scheduling heuristics and provide insights on designing new algorithms.

Task clustering [20, 31, 32, 27] merges fine-grained tasks into coarse-grained jobs. After task clustering the number of jobs is reduced and the cumulative overhead is reduced too. The low performance of *fine-grained* tasks is a common problem in widely distributed platforms where the scheduling overhead and queuing times at resources are high, such as Grid and Cloud systems. Several works have addressed the control of task granularity of bag of tasks. For instance, Muthuvelu et al. [45] proposed a clustering algorithm that groups bag of tasks based on their runtime—tasks are grouped up to the resource capacity. Later, they extended their work [46] to determine task granularity based on task file size, CPU time, and resource constraints. Recently, they proposed an online scheduling algorithm [47, 48] that groups tasks based on resource network utilization, user’s budget, and application deadline. Ng et al. [49] and Ang et al. [50] introduced bandwidth in the scheduling framework to enhance the performance of task scheduling. Longer tasks are assigned to resources with better bandwidth. Liu and Liao [51] proposed an adaptive fine-grained job scheduling algorithm to group fine-grained tasks according to processing capacity and bandwidth of the current available resources. Although these techniques significantly reduce the impact of scheduling and queuing time overhead, they are not applicable to scientific workflows, since data dependencies are not considered.

## 3. Model and Design

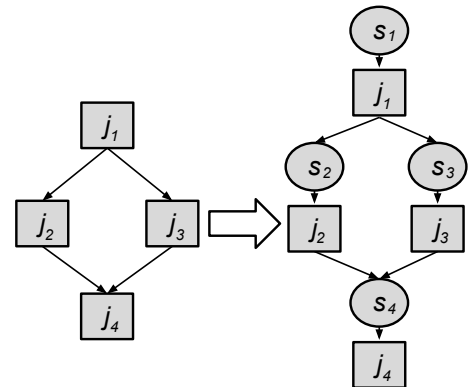


Figure 1: Extending DAG to o-DAG.

A workflow is modeled as a Directed Acyclic Graph (DAG) as shown in Fig. 1 (Left). Each node in the DAG often represents a workflow job ( $j$ ), and the edges represent dependencies between the jobs that constrain the order in which the jobs are executed. Dependencies typically represent data-flow dependencies in the application, where the output files produced by one job are used as inputs of another job. Each job is a single execution unit and it may contain one or multiple tasks, which is a program and a set of parameters that need to be executed. Fig. 1 (left) shows an illustration of a DAG composed by four jobs. This model fits several workflow management systems such as Pegasus [42], Askalon [52], and Taverna [53].

Fig. 2 shows a typical workflow execution environment. The submit host prepares a workflow for execution (clustering, mapping, etc.), and worker nodes, at an execution site, execute jobs individually. The main components are introduced below:

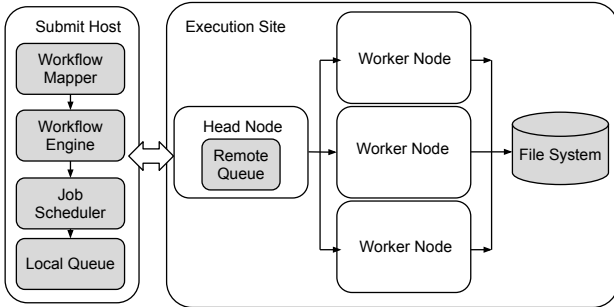


Figure 2: A workflow system model.

**Workflow Mapper.** generates an executable workflow based on an abstract workflow provided by the user or workflow composition system. It also restructures the workflow to optimize performance and adds tasks for data management and provenance information generation. In this work, workflow mapper is particularly used to merge small tasks together into a job such that system overheads are reduced, which is called Task Clustering. A job is a single execution unit in the workflow execution systems and it may contain one or more tasks.

**Workflow Engine.** executes jobs defined by the workflow in order of their dependencies. Only jobs that have all their parent jobs completed are submitted to the Job Scheduler. Workflow Engine relies on the resources (compute, storage, and network) defined in the executable workflow to perform the necessary actions. The time period when a job is free (all of its parents have completed successfully) to when it is submitted to the job scheduler is denoted the workflow engine delay. The workflow engine delay is usually configured by users to assure that the entire workflow scheduling and execution system is not overloaded.

**Job Wrapper.** extracts tasks from clustered jobs and executes them at the worker nodes. The clustering delay is the elapsed time on the extraction process.

**Job Scheduler and Local Queue.** manage individual workflow jobs and supervise their execution on local and remote resources. The time period when a job is submitted to the job scheduler to when the job starts its execution in a worker node is denoted the queue delay. It reflects both the efficiency of the job scheduler and the resource availability.

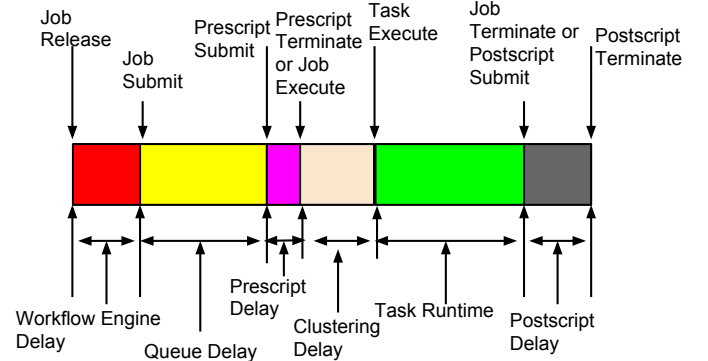


Figure 3: Workflow Events

The execution of a job is comprised of a series of events as shown in Fig. 3 and they are defined as:

1. Job Release is defined as the time when the workflow engine identifies that a job is ready to be submitted (when its parents have successfully completed).
2. Job Submit is defined as the time when the workflow engine submits a job to the local queue.
3. Job Execute is defined as the time when the workflow engine sees a job is being executed.
4. Task Execute is defined as the time when the job wrapper sees a task is being executed.
5. Pre/Postscript Start is defined as the time when the workflow engine starts to execute a pre/postscript.
6. Pre/Postscript Terminate is defined as the time when the pre/postscript returns a status code (success or failure).

Fig. 3 shows a typical timeline of overheads and runtime in a compute job. We do not specify the data transfer delay in this timeline because data transfer is handled by data transfer jobs (stage-in and stage-out jobs).

As shown in our prior work [18], we have classified workflow overheads into four categories as follows.

1. Workflow Engine Delay measures the time between when the last parent job of a job completes and the time when the job gets submitted to the local queue. The completion time of the last parent job means this job is released to the ready queue and is waiting for resources to be assigned to it. The workflow engine delay reflects the efficiency of a workflow engine (i.e., DAGMan [54]).
2. Queue Delay is defined as the time between the submission of a job by the workflow engine to the local queue and the time the local scheduler sees the job running. This overhead reflects the efficiency of the local workflow

scheduler (e.g. Condor [55]) to execute a job and the availability of resources for the execution of this job.

3. Pre/Postscript Delay is the time taken to execute a lightweight script under some execution systems before/after the execution of a job. For example, prescripts prepare working environment before the execution of a job starts and postscripts examine the status code of a job after the computational part of this job is done.
4. Clustering Delay measures the difference between the sum of the actual task runtime and the job runtime seen by the job wrapper. The cause of Clustering Delay is usually because we use a job wrapper in worker nodes to execute a clustered job that requires some delay to extract the list of tasks.

The overhead aware DAG model (o-DAG) we use in this work is an extension of the traditional DAG model. System overheads play an important role in workflow execution and constitute a major part of the overall runtime when jobs are poorly mapped to resources. Fig. 1 shows how we augment a DAG to be an o-DAG with the capability to represent system overheads ( $s$ ) such as workflow engine delay and queue delay. In summary, an o-DAG representation allows the specification of high level system overhead details, which is more suitable for the study of overhead aware scheduling.

#### 4. Overlapping Metrics

The realistic characteristics of workflows are critical to optimal workflow orchestration and profiling is an effective approach to investigate the behaviors of many complex applications. In this paper, we particularly focus on the overlapped and cumulative overheads of workflow events because this approach represents a promising trend of optimizing workflows and there is a lack of supporting analysis tools.

Workflow is typically a graph of computational activities, data transfer and system overheads as shown in our o-DAG model. Different branches of these activities may overlap with each other in the timeline and our major concern is their cumulative projection on the timeline or makespan. People have been exploring on new approaches to overlap these overheads without the necessity of reducing them. However, the challenge is how these overlapped activities contribute to the eventual makespan and how to reveal their overlapping effects in timeline from different aspects.

Fig. ?? shows the timeline of the workflow in Fig. 1. In this simple example, we are interested in questions such as: (1) whether the workflow engine delay has a good overlapping within itself? (2) whether the queue delay has a good overlapping with other types of overheads? (3) whether those 'bottleneck' overheads have overlapped with others? In the rest of this section, we will use this workflow as an example to show how we implement these metrics.

##### 4.1. Metrics to Evaluate Cumulative Overheads and Runtimes

In this section, we propose four metrics to calculate cumulative overheads of workflows, which are *Sum*, *Projection(PJ)*,

*Exclusive Projection(EP)* and *Impact Factor(IF)*. *Sum* simply adds up the overheads of all jobs without considering their overlap. *PJ* subtracts from *Sum* all overlaps of the same type of overhead. It is equal to the projection of all overheads to the timeline. *EP* subtracts the overlap of all types of overheads from *PJ*. It is equal to the projection of overheads of a particular type excluding all other types of overheads to the timeline. *IF* uses a reverse ranking algorithm to index overheads and then calculates the cumulative overhead weighted by the ranks (impact factors). The idea is brought by web page indexing algorithms such as PageRank [56]. The calculation of *Sum*, *PJ* and *EP* is straightforward and Fig. 5 shows how to calculate the impact factor (*IF*) of the same workflow graph in Fig. 4. Both *PJ* and *EP* are proposed to answer Questions (1) and (2) and *IF* answers Question (3), while *Sum* serves as a comparison for them.

$$IF(j_u) = d + (1 - d) \times \sum_{j_v \in Child(j_u)} \frac{IF(j_v)}{\|Parent(j_v)\|} \quad (1)$$

Equation 1 means that the *IF* of a node (overhead or job runtime) is determined by the *IF* of its child nodes.  $d$  is the damping factor, which controls the speed of the decrease of the *IF*.  $\|Parent(j_v)\|$  is the number of parents that node  $j_v$  has. Intuitively speaking, a node is more important if it has more children and/or its children are more important. In terms of workflows, it means an overhead has more power to control the release of other overheads and computational activities. There are two differences compared to the original PageRank:

1. We use output link pointing to child nodes while PageRank uses input link from parent nodes, which is why we call it reverse ranking algorithm.
2. Since a workflow is a DAG, we do not need to calculate *IF* iteratively. For simplicity, we assign the *IF* of the root node to be 1. And then we calculate the *IF* of a workflow ( $G$ ) based on the equation below, while  $\phi_{j_u}$  indicates the duration of node  $j_u$ .

$$IF(G) = \sum IF(j_u) \times \phi_{j_u} \quad (2)$$

*IF* has two important features: (1) *IF* of a node indicates the importance of this node in the whole workflow graph and its likelihood to be a bottleneck, the greater the more important; (2) *IF* decreases from the top of the workflow to down, the speed of which is controlled by the damping factor  $d$ . It reflects the intuition that the overhead occurred at the beginning of the workflow execution is likely to be more important than that at the end. By analyzing these four types of cumulative overheads, researchers have a clearer view of whether their optimization methods have overlapped the overheads of a same type (if  $PJ < Sum$ ) or other types (if  $EP < PJ$ ). Besides importance, *IF* is also able to show the connectivity within the workflow, the larger the denser. We use a simple example workflow with four jobs to show how to calculate the overlap and cumulative overheads. Fig. 4 shows the timeline of our example workflow.  $j_1$  and  $j_4$  are the parent and children of  $j_2$  and  $j_3$  respectively.

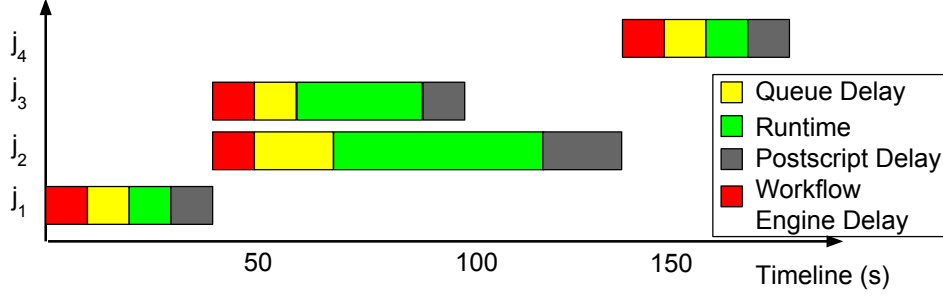


Figure 4: Workflow Timeline

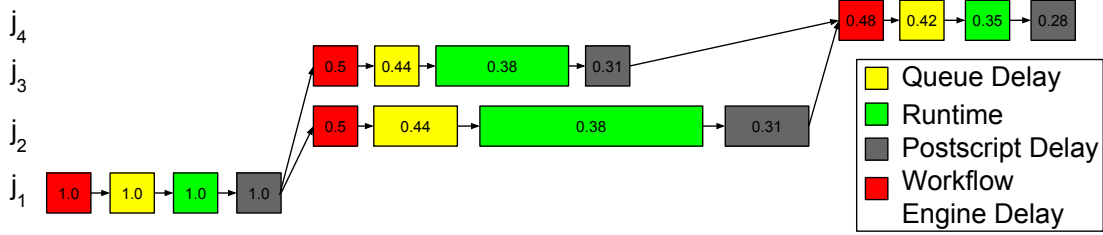


Figure 5: Impact Factor

Table 1: Overhead and Runtime Information

Job	Release Time	Queue Delay	Workflow Engine Delay	Runtime	Postscript Delay
$j_1$	0	10	10	10	10
$j_2$	40	10	20	50	20
$j_3$	40	10	10	30	10
$j_4$	150	10	10	10	10

At  $t=0$ ,  $j_1$  is first released and once it is done at  $t=40$ ,  $j_3$  and  $j_2$  are released. Finally, at  $t=140$ ,  $j_4$  is released. Table. 1 shows their overhead and runtime duration (assuming). For example,  $PJ$  of queue delay is 40 since the queue delay of  $j_2$  and  $j_3$  overlaps from  $t=50$  to 60.  $EP$  of queue delay is 10 less than  $PJ$  of queue delay since the queue delay of  $j_2$  overlaps with the runtime of  $j_3$  from  $t=60$  to 70.

For simplicity, we do not include the data transfer delay, pre-script delay and others. The overall makespan for this example workflow is 180. Table 2 shows the percentage of overheads and job runtime over makespan.

Table 2: Percentage of Overheads and Runtime

Contribution	Sum	PJ	EP	IF
runtime(%)	57.1	42.8	28.5	17.7
queue delay(%)	28.5	21.4	14.2	13.0
workflow engine delay(%)	21.4	14.2	14.2	14.2
postscript delay(%)	28.5	28.5	21.4	11.2

In Table 2, we can conclude that the sum of  $Sum$  is larger than makespan and smaller than  $makespan \times (\text{number of resources})$  because it does not count the overlap at all.  $PJ$  is larger than makespan since the overlap between more than two types

of overheads may be counted twice or more.  $EP$  is smaller than makespan since some overlap between more than two types of overheads may not be counted.  $RR$  shows how intensively these overheads and computational activities are connected to each other.

#### 4.2. Experiments and Evaluations

We applied these four metrics to a widely used workflow in our experiments. These workflows were run on distributed platforms including clouds, grids and dedicated clusters. On clouds, virtual machines were provisioned and then the required services (such as file transfer services) were deployed. We examined two clouds: Amazon EC2 [57] and FutureGrid [58]. Amazon EC2 is a commercial, public cloud that is been widely used in distributed computing. We examined the overhead distributions of a widely used astronomy workflow called Montage [59] that is used to construct large image mosaics of the sky. Montage was run on FutureGrid [58]. FutureGrid is a distributed, high-performance testbed that provides scientists with a set of computing resources to develop parallel, grid, and cloud applications.

### 4.3. Relationship between Overhead Metrics and Overall Performance

In this section, we aim to investigate the relationship between the overhead metrics that we proposed and the overall performance of popular workflow restructuring techniques. Among them, task clustering [60] is a technique that increases the computational granularity of tasks by merging small tasks together into a clustered job, reducing the impact of the queue wait time and also the makespan of the workflow. Data or job throttling [28] limits the amount of parallel data transfer to avoid overloading supporting services such as data servers. Throttling is especially useful for unbalanced workflows in which one task might be idle while waiting for data to arrive. The aim of throttling is to appropriately regulate the rate of data transfers between the workflow tasks via data transfer servers by ways of restricting the data connections, data threads or data transfer jobs. Provisioning tools often deploy pilot jobs as placeholders for the execution of application jobs. Since a placeholder can allow multiple application jobs to execute during its lifetime, some job scheduling overheads can be reduced.

#### 4.3.1. How Task Clustering Reduces Overheads

Metric	Workflow Engine Delay	Queue Delay	Runtime
SUM	$1.5 \times 10^5$	$1.9 \times 10^7$	$1.5 \times 10^6$
SUM/n	54(0.16%)	$6.8 \times 10^3$ (20%)	515(1.6%)
PJ	$3.2 \times 10^3$ (9.3%)	$2.9 \times 10^4$ (85%)	$3.3 \times 10^4$ (102%)
EP	70(0.2%)	665(1.9%)	$4.5 \times 10^3$ (14%)
IF	310(0.9%)	$1.6 \times 10^4$ (45%)	$3.1 \times 10^3$ (9.4%)

Table 3: Metrics Without Task Clustering

Metric	Workflow Engine Delay	Queue Delay	Runtime
SUM	681(74%)	$1.0 \times 10^3$ (112%)	$4.4 \times 10^3$ (475%)
SUM/n	6.6(0.72%)	10(1.1%)	43(4.6%)
PJ	116(13%)	197(21%)	660(72%)
EP	72(7.8%)	90(9.8%)	420(46%)
IF	117(13%)	165(18%)	442(48%)

Table 4: Metrics with Task Clustering

In the following sections, we use a Montage workflow to show how different optimization methods improve overall performance. Many workflows are composed of thousands of fine computational granularity tasks. Task clustering is a technique that increases the computational granularity of tasks by merging small jobs together into a clustered job, reducing the impact of the queue wait time and minimizing the makespan of the workflow. Table. 4 and Table. 3 compare the overheads and runtime of the Montage workflow.  $SUM/n$  indicates the average overhead or runtime per job. The percentage is calculated by the cumulative overhead ( $PJ$ ,  $EP$  or  $IF$ ) divided by the makespan of workflows. In this example, we can see that  $PJ$ ,  $EJ$  and  $IF$  consistently show that the portion of runtime is increased compared to overheads with task clustering. For example, the  $IF$  of queue delay without clustering (45%) is much larger than the  $IF$  of runtime (9.4%). In the case of task clustering, the  $IF$  of runtime (48%) is much larger than the  $IF$  of queue delay (18%). We can conclude that task clustering improves the runtime performance by reducing the influence of

queue delay (more specifically, overlapping). The metric  $SUM$  and  $SUM/n$ , which are usually used in other work, do not provide useful insight for us.

#### 4.3.2. How Job Throttling Reduces Overheads

Metric	Workflow Engine Delay	Queue Delay	Runtime
SUM	$9.2 \times 10^4$	$1.7 \times 10^5$	$9.2 \times 10^3$
SUM/n	32(2.6%)	60(4.8%)	3.2(0.3%)
PJ	558(44.6%)	873(70%)	990(79%)
EP	84(6.7%)	90(7.2%)	190(15.2%)
IF	162(13%)	331(27%)	205(16.4%)

Table 5: Metrics with Throttling ( $p=24$ )

Metric	Workflow Engine Delay	Queue Delay	Runtime
SUM	$7.4 \times 10^4$	$1.6 \times 10^5$	$6.5 \times 10^3$
SUM/n	25.9(2.2%)	57(4.9%)	2.3(0.2%)
PJ	561(47.5%)	856(72.5%)	928(78.6%)
EP	77(6.5%)	75(6.4%)	140(11.9%)
IF	153(13%)	307(26%)	187(15.8%)

Table 6: Metrics with Throttling ( $p=16$ )

Metric	Workflow Engine Delay	Queue Delay	Runtime
SUM	$9.2 \times 10^4$	$1.7 \times 10^5$	$9.2 \times 10^3$
SUM/n	32(2.5%)	59(4.7%)	3.2(0.3%)
PJ	520(41%)	896(71%)	1073(85%)
EP	75(5.9%)	70(5.5%)	185(14.6%)
IF	142(11.2%)	326(25.7%)	223(17.6%)

Table 7: Metrics with Throttling ( $p=12$ )

Data or job throttling limits the amount of parallel data transfer to avoid overloading supporting services such as data servers. Throttling is especially useful for unbalanced workflows in which one task might be idle while waiting for data to arrive. The aim of throttling is to appropriately regulate the rate of data transfers between the workflow tasks via data transfer servers by ways of restricting the data connections, data threads or data transfer jobs. Especially on cloud platforms, I/O requests need to go through more layers than a physical cluster; and thereby workflows may suffer a higher overhead from data servers.

In our experiments, the data transfer service is deployed on a virtual machine that is similar to a worker node. In this section, we evaluate a simple static throttling strategy where the Condor scheduler limits the number of concurrent jobs to be run and thereby restricts the number of parallel I/O requests. There are 32 resources available and we evaluate the cases with throttling parameters ( $p$ , the maximum jobs in queue) that are equal to 24, 16 and 12 respectively. In the case of  $p=24$ , the resources are better utilized but the data server is heavily loaded. In the case of  $p=12$ , the resources are under-utilized even though the data server has more capabilities. Table. ?? show the contribution of workflow overheads and runtime. With limited throttling (reducing threshold from 24 to 16), the data transfer requests are distributed in the timeline more evenly and, as a result, their overhead is reduced. However, with over throttling (reducing threshold from 16 to 12), resources are not fully utilized and thus the makespan is increased. In this experiment,  $PJ$ ,  $EP$  and  $IF$  reflect the variation trend of overheads and makespan better than  $SUM$  and  $SUM/n$ .

### 4.3.3. How Provisioning Reduces Overheads

Metric	Workflow Engine Delay	Queue Delay	Runtime
SUM	$1.5 \times 10^5$	$1.9 \times 10^7$	$1.5 \times 10^6$
SUM/n	54(0.16%)	$6.8 \times 10^3$ (20%)	515(1.6%)
PJ	$3.2 \times 10^3$ (9.3%)	$2.9 \times 10^4$ (85%)	$3.3 \times 10^4$ (102%)
EP	70(0.2%)	665(1.9%)	$4.5 \times 10^3$ (14%)
IF	310(0.9%)	$1.6 \times 10^4$ (45%)	$3.1 \times 10^3$ (9.4%)

Table 8: Metrics Without Resource Provisioning

Metric	Workflow Engine Delay	Queue Delay	Runtime
SUM	$8.1 \times 10^4$	$5.0 \times 10^5$	$3.1 \times 10^4$
SUM/n	28(0.9%)	173(5.5%)	11(0.4%)
PJ	$1.0 \times 10^3$ (32%)	$2.3 \times 10^3$ (74%)	$3.0 \times 10^3$ (94%)
EP	73(2.3%)	50(1.6%)	588(19%)
IF	174(5.5%)	840(27%)	683(22%)

Table 9: Metrics with Resource Provisioning

Many of the scientific applications presented here consist of a large number of short-duration tasks whose runtimes are greatly influenced by overheads present in distributed environments. Most of these environments have an execution mode based on batch scheduling where jobs are held in a queue until resources become available to execute them. Such a best-effort model normally imposes heavy overheads in scheduling and queuing. For example, Condor-G [55] uses Globus GRAM [61] to submit jobs to remote clusters. The Globus Toolkit normally has a significant overhead compared to running Condor directly as an intra domain resource and job management system. Provisioning tools often deploy pilot jobs as placeholders for the execution of application jobs. Since a placeholder can allow multiple application jobs to execute during its lifetime, some job scheduling overheads can be reduced. In our experiments, we compared the performance of Condor-G (without provisioning) and Corral (with provisioning).

Table. 8 and Table. 9 show the contribution of workflow overheads and runtime. The percentage is calculated by the cumulative overhead (*PJ*, *EP*, or *IF*) divided by the makespan of workflows. Comparing *PJ*, *EP* and *IF*, we can conclude that the overheads with provisioning have been reduced significantly. The reason is that the local scheduler has direct control over the resources without going through Globus.

## 5. Imbalance Metrics

With an o-DAG model, we can explicitly express the process of task clustering. For instance, in Fig. 3, two tasks *t1* and *t2*, without data dependency between them, are merged into a clustered job *j1*. A job *j* is a single execution unit composed by one or multiple task(s). Job wrappers are commonly used to execute clustered jobs, but they add a overhead denoted the clustering delay *c*. Clustering delay measures the difference between the sum of the actual task runtimes and the job runtime seen by the job scheduler. After horizontal clustering, *t1* and *t2* in *j1* can be executed in sequence or in parallel, if supported. In this paper, we consider sequential executions only. Given a single resource, the overall runtime for the workflow in Fig. 3 (left) is  $\text{runtime1} = s1 + t1 + s2 + t2$ , and the overall runtime for

the clustered workflow in Fig. 3 (right) is  $\text{runtime2} = s1 + c1 + t1 + t2$ .  $\text{runtime1} \geq \text{runtime2}$  as long as  $c1 \leq s2$ , which is the case of many distributed systems since the clustering delay within an execution node is usually shorter than the scheduling overhead across different execution nodes. Fig 3 shows a typical example of a Horizontal Clustering.

Fig. 3: An Example of Task Clustering.

(HC) technique that groups tasks at the same horizontal level. In our work, we define the level of a task as the longest depth from the root task to this task (Depth First Search) because the longest depth controls the final release of this task.

Task clustering has been widely used to group fine-grained tasks into coarse-grained jobs [45, 46, 47, 48, 49, 50, 51, 62]. However, the challenge of balancing the runtime imbalance and dependency imbalance is still not yet addressed.

In a scientific workflow, tasks within a level (or depth within a workflow directed acyclic graph) may have different runtimes. Merging tasks within a level without considering the runtime variance may cause load imbalance, i.e., some clustered jobs may be composed of short running tasks while others of long running tasks. This imbalance delays the release of tasks from the next level of the workflow, penalizing the workflow execution with an overhead produced by the use of inappropriate task clustering strategies [63].

In another way, data dependencies between workflow tasks play an important role when clustering tasks within a level. A data dependency means that there is a data transfer between two tasks (output data for one and input data for the other). Grouping tasks without considering these dependencies may lead to data locality problems where output data produced by parent tasks are poorly distributed. Thus, data transfer times and failures probability increase.

However, what makes it even difficult is there is a tradeoff between runtime and data dependency balancing. For instance, balancing runtime may aggravate the dependency imbalance problem, and vice versa. A quantitative measurement of workflow characteristics is required to serve as a criterion to select and balance these solutions. To achieve this goal, we propose a series of metrics that reflect the internal structure (in terms of task runtimes and dependencies) of the workflow and introduce balancing methods based on these metrics to address these challenges.

In particular, we provide a novel approach to capture these metrics. Traditionally, there are two approaches to improve the performance of task clustering. The first one is a top-down approach [64] that represents the clustering problem as a global optimization problem and aims to minimize the overall workflow execution time. However, the complexity of solving such an optimization problem does not scale well since most methods use genetic algorithms. The second one is a bottom-up approach [45, 51] that only examines free tasks to be merged and optimizes the clustering results locally. In contrast, our work extends these approaches to consider the neighboring tasks including siblings, parents, and children because such a family of tasks has strong connections between them.



### 5.1. Imbalance Metrics

**Runtime Imbalance** describes the difference of the task/job runtime of a group of tasks/jobs. In this work, we denote the **Horizontal Runtime Variance (HRV)** as the ratio of the standard deviation in task runtime to the average runtime of tasks/jobs at the same horizontal level of a workflow. At the same horizontal level, the job with the longest runtime often controls the release of the next level jobs. A high *HRV* value means that the release of next level jobs has been delayed. Therefore, to improve runtime performance, it is meaningful to reduce the standard deviation of job runtime. Fig. 6 shows an example of four independent tasks  $t_1$ ,  $t_2$ ,  $t_3$  and  $t_4$  where task runtime of  $t_1$  and  $t_2$  is half of that of  $t_3$  and  $t_4$ . In the Horizontal Clustering (HC) approach, a possible clustering result could be merging  $t_1$  and  $t_2$  into a clustered job and  $t_3$  and  $t_4$  into another. This approach results in imbalanced runtime, i.e.,  $HRV > 0$  (Fig. 6-top). In contrast, a balanced clustering strategy should try its best to evenly distribute task runtime among jobs as shown in Fig. 6 (bottom). Generally speaking, a smaller *HRV* means that the runtime of tasks at the same horizontal level is more evenly distributed and therefore it is less necessary to balance the runtime distribution. However, runtime variance is not able to describe how regular is the structure of the dependencies between the tasks.

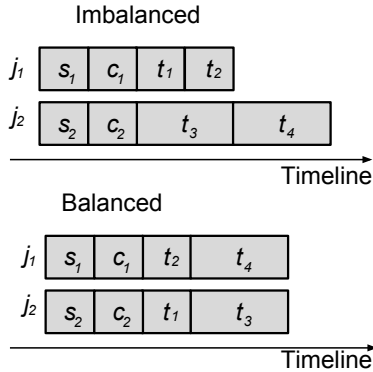


Figure 6: An Example of Runtime Variance.

**Dependency Imbalance** means that the task clustering at one horizontal level forces the tasks at the next level (or even subsequent levels) to have severe data locality problem and thus loss of parallelism. For example, in Fig. 7, we show a two-level workflow composed of four tasks in the first level and two in the second. Merging  $t_1$  with  $t_2$  and  $t_3$  with  $t_4$  (imbalanced workflow in Fig. 7) forces  $t_5$  and  $t_6$  to transfer files from two locations and wait for the completion of  $t_1$ ,  $t_2$ ,  $t_3$ , and  $t_4$ . A balanced clustering strategy groups tasks that have the maximum number of child tasks in common. Thus,  $t_5$  can start to execute as soon as  $t_1$  and  $t_3$  are completed, and so can  $t_6$ . To measure and quantitatively demonstrate the Dependency Imbalance of a workflow, we propose two metrics: (i) Impact Factor Variance, and (ii) Distance Variance.

We define the **Impact Factor Variance (IFV)** of tasks as the standard deviation of their impact factor. The intuition behind

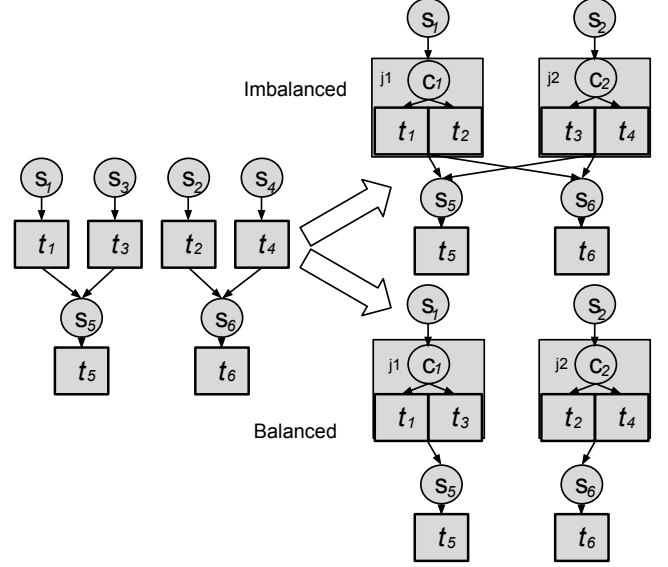


Figure 7: An Example of Dependency Variance.

the Impact Factor is that we aim to capture the similarity of tasks/jobs in a graph by measuring their relative impact factor or importance to the entire graph. Intuitively speaking, tasks with similar impact factors should be merged together compared to tasks with different impact factors. Also, if all the tasks have similar impact factors, the workflow structure tends to be more ‘even’ or ‘regular’. The **Impact Factor (IF)** of a task  $t_u$  is defined as follows:

$$IF(t_u) = \sum_{t_v \in \text{Child}(t_u)} \frac{IF(t_v)}{\|\text{Parent}(t_v)\|} \quad (3)$$

where  $\text{Child}(t_u)$  denotes the set of child tasks of  $t_u$ , and  $\|\text{Parent}(t_v)\|$  the number of parent tasks of  $t_v$ . Compared to Eq. 1, the difference is that we set the damping factor to be 0 since we are doing horizontal clustering and thus there is no need to differentiate the level of a task. For simplicity, we assume the *IF* of a workflow exit task (e.g.  $t_5$  in Fig. 7) as 1.0. For instance, consider the two workflows presented in Fig. 8. *IF* for  $t_1$ ,  $t_2$ ,  $t_3$ , and  $t_4$  are computed as follows:

$$\begin{aligned} IF(t_7) &= 1.0, IF(t_6) = IF(t_5) = IF(t_7)/2 = 0.5 \\ IF(t_1) &= IF(t_2) = IF(t_5)/2 = 0.25 \\ IF(t_3) &= IF(t_4) = IF(t_6)/2 = 0.25 \end{aligned}$$

Thus,  $IFV(t_1, t_2, t_3, t_4) = 0$ . In contrast, *IF* for  $t'_1$ ,  $t'_2$ ,  $t'_3$ , and  $t'_4$  are:

$$\begin{aligned} IF(t'_7) &= 1.0, IF(t'_6) = IF(t'_5) = IF(t'_1) = IF(t'_7)/2 = 0.5 \\ IF(t'_2) &= IF(t'_3) = IF(t'_4) = IF(t'_6)/3 = 0.17 \end{aligned}$$

Therefore, the *IFV* value for  $t'_1$ ,  $t'_2$ ,  $t'_3$ ,  $t'_4$  is 0.17, which means it is less regular than the workflow in Fig. 8 (left). In this work,

we use **HIFV** (Horizontal IFV) to indicate the *IFV* of tasks at the same horizontal level. The time complexity of calculating all the *IF* of a workflow with  $n$  tasks is  $O(n)$ .

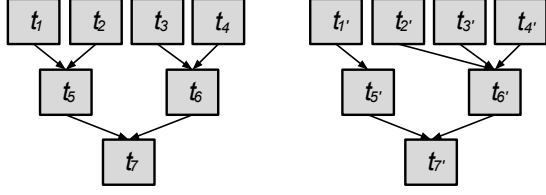


Figure 8: Example of workflows with different data dependencies.

**Distance Variance (DV)** describes how ‘closely’ tasks are to each other. The distance between two tasks/jobs is defined as the cumulative length of the path to their closest common successor. If they do not have a common successor, the distance is set to infinity. For a group of  $n$  tasks/jobs, the distance between them is represented by a  $n \times n$  matrix  $D$ , where an element  $D(u, v)$  denotes the distance between a pair of tasks/jobs  $u$  and  $v$ . For any workflow structure,  $D(u, v) = D(v, u)$  and  $D(u, u) = 0$ , thus we ignore the cases when  $u \geq v$ . Distance Variance is then defined as the standard deviation of all the elements  $D(u, v)$  for  $u < v$ . The time complexity of calculating all the  $D$  of a workflow with  $n$  tasks is  $O(n^2)$ .

Similarly, *HDV* indicates the *DV* of a group of tasks/jobs at the same horizontal level. For example, Table 10 shows the distance matrices of tasks from the first level for both workflows of Fig. 8 ( $D_1$  for the workflow in the left and  $D_2$  for the workflow in the right). *HDV* for  $t_1, t_2, t_3$ , and  $t_4$  is 1.03, and for  $t'_1, t'_2, t'_3$ , and  $t'_4$  is 1.10. In terms of distance variance,  $D_1$  is more ‘even’ than  $D_2$ . Intuitively speaking, a smaller *HDV* means the tasks at the same horizontal level are more equally ‘distant’ to each other and thus the workflow structure tends to be more ‘evenly’ and ‘regular’.

In conclusion, runtime variance and dependency variance offer a quantitative and comparable tool to measure and evaluate the internal structure of a workflow.

$D_1$	$t_1$	$t_2$	$t_3$	$t_4$	$D_2$	$t'_1$	$t'_2$	$t'_3$	$t'_4$
$t_1$	0	2	4	4	$t'_1$	0	4	4	4
$t_2$	2	0	4	4	$t'_2$	4	0	2	2
$t_3$	4	4	0	2	$t'_3$	4	2	0	2
$t_4$	4	4	2	0	$t'_4$	4	2	2	0

Table 10: Distance matrices of tasks from the first level of workflows in Fig. 8.

## 5.2. Balanced Clustering Methods

In this subsection, we introduce our balanced clustering methods used to improve the runtime balance and dependency balance in task clustering. We first introduce the basic runtime-based clustering method and then two other balancing methods that address the dependency imbalance problem. We use the

metrics presented in the previous subsection to evaluate a given workflow to decide which balancing method(s) is(are) more appropriate.

Algorithm 1 shows the pseudocode of our balanced clustering algorithm that uses a combination of these balancing methods and metrics. The maximum number of clustered jobs (size of  $CL$ ) is equal to the number of available resources multiplied by a *clustering factor*.

### Algorithm 1 Balanced Clustering algorithm

---

**Require:**  $W$ : workflow;  $CL$ : list of clustered jobs;  $C$ : the required size of  $CL$ ;  
**Ensure:** The job runtime of  $CL$  are as even as possible

```

1: procedure CLUSTERING( $W, D, C$ )
2:   Sort  $W$  in decreasing order of the size of each level
3:   for level < the depth of  $W$  do
4:      $TL \leftarrow \text{GETTASKSATLEVEL}(w, \text{level})$   $\triangleright$  Partition  $W$  based on depth
5:      $CL \leftarrow \text{MERGE}(TL, C)$   $\triangleright$  Form a list of clustered jobs
6:      $W \leftarrow W - TL + CL$   $\triangleright$  Merge dependencies as well
7:   end for
8: end procedure
9: procedure MERGE( $TL, C$ )
10:  Sort  $TL$  in decreasing order of task runtime
11:  for  $t$  in  $TL$  do
12:     $J \leftarrow \text{GETCANDIDATEJOB}(CL, t)$   $\triangleright$  Get a candidate task
13:     $J \leftarrow J + t$   $\triangleright$  Merge it with the clustered job
14:  end for
15:  return  $CL$ 
16: end procedure
17: procedure GETCANDIDATEJOB( $CL, t$ )
18:  Selects a job based on balanced clustering methods
19: end procedure

```

---

We examine tasks in a level-by-level approach starting from the level with the largest width (number of tasks at the same level, line 2). The intuition behind this breadth favored approach is that we believe it should improve the performance most. Then, we determine which type of imbalance problem a workflow experiences based on the balanced clustering metrics presented previously (*HRV*, *HIFV*, and *HDV*), and accordingly, we select a combination of balancing methods. *GETCANDIDATEJOB* selects a job (line 12) from a list of potential candidate jobs ( $CL$ ) to be merged with the targeting task ( $t$ ). Below we introduce the three balancing methods proposed in this work.

**Horizontal Runtime Balancing (HRB)** aims to evenly distribute task runtime among jobs. Tasks with the longest runtime are added to the job with the shortest runtime. This greedy method is used to address the imbalance problem caused by runtime variance at the same horizontal level. Fig. 9 shows how HRB works in an example of four jobs with different job runtime (assuming the height of a job is its runtime). For the given task ( $t_0$ ), HRB sorts the potential jobs ( $j_1, j_2, j_3$ , and  $j_4$ ) based on their runtime and selects the shortest job (in this case  $j_1$  or  $j_2$ ).

However, HRB may cause a dependency imbalance problem since the clustering does not take data dependency into consideration. To address this problem, we propose the **Horizontal Impact Factor Balancing (HIFB)** and the **Horizontal Distance Balancing (HDB)** methods.

In HRB, candidate jobs are sorted by their runtime, while in HIFB jobs are first sorted based on their similarity of *IF*, then

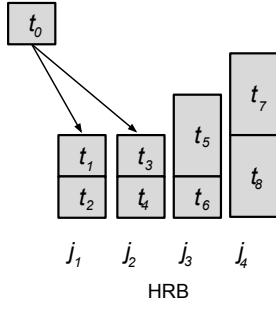


Figure 9: An example of HRB.

on runtime. For example, in Fig. 10, assuming 0.2, 0.2, 0.1, and 0.1 IF values of  $j_1$ ,  $j_2$ ,  $j_3$ , and  $j_4$  respectively, HIFB selects a list of candidate jobs with the same IF value, i.e.  $j_3$  and  $j_4$ . Then, HRB is performed to select the shortest job ( $j_3$ ).

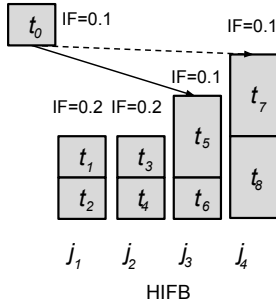


Figure 10: An example of HIFB.

Similarly, in HDB jobs are sorted based on the distance between them and the targeted task  $t_0$ , then on their runtimes. For instance, in Fig. 11, assuming 2, 4, 4, and 2 the distances to  $j_1$ ,  $j_2$ ,  $j_3$ , and  $j_4$  respectively, HDB selects a list of candidate jobs with the minimal distance ( $j_1$  and  $j_4$ ). Then, HRB is performed to select the shortest job ( $j_1$ ).

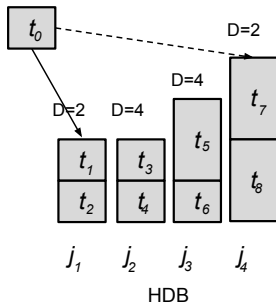


Figure 11: An example of HDB.

In conclusion, these balancing methods have different preference on the selection of a candidate job to be merged with the targeting task. HIFB tends to group tasks that share similar position/importance to the workflow structure. HDB tends to

group tasks that are closed to each other to reduce data transfers.

### 5.3. Experiment Conditions

The experiments presented hereafter evaluate the performance of our balancing methods in comparison with an existing and effective task clustering strategy named Horizontal Clustering (HC) [65], which is widely used by workflow management systems such as Pegasus.

We extended the WorkflowSim [66] simulator with the balanced clustering methods and imbalance metrics to simulate a distributed environment where we could evaluate the performance of our methods when varying the average data size and task runtime. The simulated computing platform is composed by 20 single homogeneous core virtual machines (worker nodes), which is the quota per user of some typical distributed environments such as Amazon EC2 [67] and FutureGrid [58]. Each machine has 512MB of memory and the capacity to process 1,000 million instructions per second. Task scheduling is data-aware, i.e. tasks are scheduled to resources which have the most input data available.

Two workflows are used in the experiments: LIGO [68] inspiral analysis, and Epigenomics [69]. Both workflows are generated and varied using the WorkflowGenerator<sup>1</sup>. LIGO is composed by 400 tasks and its workflow structure is presented in Fig. 12 (top); Epigenomics has about 500 tasks and is structured as showed in Fig. 12 (bottom). Runtime (average and task runtime distribution) and overhead (workflow engine delay, queue delay, and network bandwidth) information were collected from real traces production environments [18, 8], then used as input parameters for the simulations. We randomly select 20% from LIGO workflow tasks and increase their task runtime by a factor of *Ratio* to simulate the system variation in a production environment. As we have mentioned in Subsection 5.2, the maximum number of clustered jobs is equal to the number of available resources multiplied by a *clustering factor*. Similar to [26], we use *clustering factor* = 2 in the experiments conducted in this work.

Two sets of experiments are conducted.

Experiment 1 evaluates the reliability and the influence of average data size in our balancing methods, since data has becoming more and more intensive in scientific workflows [8]. In this experiment set, there is no runtime variance ( $HRV = 0$ ). The original average data size (both input and output data) of the LIGO workflow is about 5MB, and of the Epigenomics workflows is about 45MB. We increase the average data size up to 5GB.

Experiment 2 evaluates the influence of the runtime variation ( $HRV$ ) in our balancing methods. We assume a normal distribution to vary task runtimes based on average and standard deviation. In this experiment set, there is no variation on the data size.

Simulation results present a confidence level of 95%. We define the performance gain over HC ( $\mu$ ) as the performance of

<sup>1</sup><https://confluence.pegasus.isi.edu/display/pegasus/WorkflowGenerator>

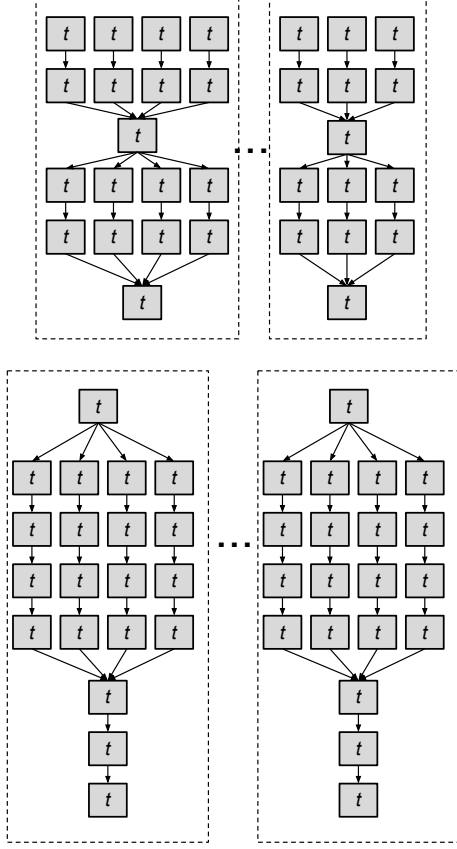


Figure 12: A simplified visualization of the LIGO Inspirar workflow (top) and Epigenomics workflow (bottom).

the balancing methods related to the performance of Horizontal Clustering (HC). Thus, for values of  $\mu > 0$  our balancing methods perform better than the HC method. Otherwise, the balancing methods perform poorer.

#### 5.4. Results and Discussion

Experiment 1: Fig. 13 (top) shows the performance gain over HC  $\mu$  of the balancing methods compared to the HC method for the LIGO workflow. HIFB and HDB significantly increase the performance of the workflow execution. Both strategies capture the structural and runtime information, reducing data transfers between tasks, while HRB focuses on runtime distribution, which in this case is none. Fig. 13 (bottom) shows the performance of the balancing methods for the Epigenomics workflow. When increasing the average data size, only HDB demonstrates significantly improvement related to HC. Investigating the structure of the Epigenomics workflow (Fig. 12-bottom), we can see that all tasks at the same horizontal level share the same IFs ( $HIFV = 0$ ), because each branch (surrounded by dash lines) happen to have the same amount of pipelines. Thus, HIFB has no performance improvement when compared to HC. However, for LIGO (Fig. 12-top),  $HIFV \neq 0$ , thus HIFB improves the workflow runtime performance. HDB captures the strong connections between tasks (data dependencies) and HIFB captures the weak connections (similarity in terms

of structure). In both workflows,  $HDV$  is not zero thus HDB performs better than HC.

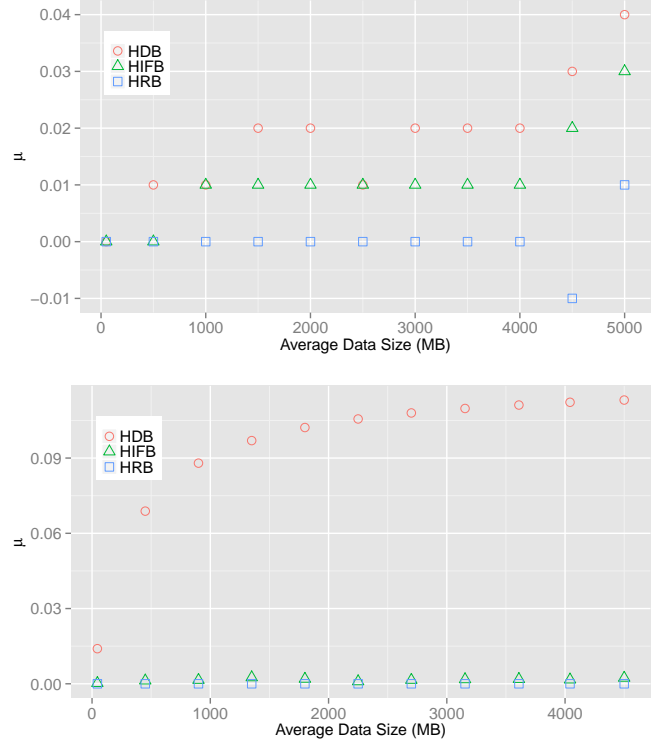


Figure 13: Experiment 1: Performance of the LIGO workflow (top) and the Epigenomics workflow (bottom).

Experiment 2: Fig. 14 shows the performance gain  $\mu$  when varying task runtimes for the LIGO workflow. As expected, when  $HRV$  increases HRB over performs HC. However, HDB and HIFB demonstrate poor performance because they merge tasks based on data dependencies first, and then, they balance the runtime distribution. For high values of  $HRV$ , we just simply need to use HRB. Otherwise, we can use either HDB or HIFB while in some cases HIFB fails to capture the structural information.

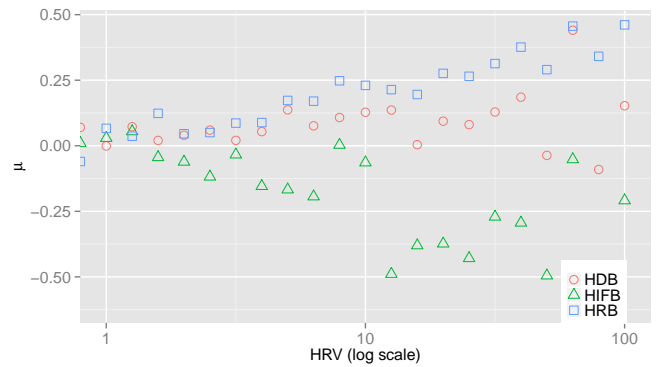


Figure 14: Experiment 2: Influence of  $HRV$  (LIGO workflow).

## 6. Sensitivity Metrics

Many computational scientists develop and use large-scale, loosely-coupled applications that are often structured as scientific workflows, which consist of many computational tasks with data dependencies between them. When executing these applications on a multi-machine distributed environment, such as the Grid or the Cloud, significant system overheads may exist [18, 19, 24, 35, 66] and the problem of choosing robust schedules becomes more and more important. Traditionally, a carefully crafted schedule is based on deterministic or statistic estimates for the execution time of computational activities that compose a workflow. However, in such an environment, this approach may prove to be grossly inefficient [66], as a result of various unpredictable overheads that may occur at runtime. Thus, to mitigate the impact of uncertain overheads, it is necessary to choose a schedule that guarantees overhead robustness, that is, a schedule that is affected as little as possible by various overhead changes.

There are several ways to achieve overhead robustness. A first approach is to integrate the overhead estimation into the job scheduling problem. A static or statistic estimation of communication cost or data transfer delay [24, 35] has been considered in the scheduling problem. Once we have the deterministic or statistic information of overheads, we can treat the system overhead as computational activities and the goal is to minimize the overall runtime including overhead duration. However, this approach only applies to the estimation of data transfer delay since the highly unpredictable variability and variety of other overheads make it a challenging work and not efficient in practice. Our prior work [18] has shown the variation of overheads may be comparable to the job runtime and thus makes it unrealistic in a real environment.

A significant amount of work [39, 24, 35] in the literature has focused on proposing algorithms that are aware of the dynamic changes of runtime environments. Task rescheduling [70, 71] is a typical approach that dynamically allocates tasks to an idle processor in order to take into account information that has been made available during the execution. Specifically, resource load [24] can be used to estimate the variance. However, rescheduling a task is costly as it implies some extra communication and synchronization costs. Relevant studies [70] indicate that it is important to have a static schedule with good properties before the start of the execution. Therefore, even if a dynamic strategy is used, a good initial placement would reduce the possibility of making a bad decision.

Another approach is to overestimate the execution time of individual jobs. Delay scheduling [72] waits for a small amount of time, letting other MapReduce jobs launch tasks instead and this method can achieve a better tradeoff of locality and fairness. However, this method only applies to workload scheduling and particularly MapReduce jobs since the duration of them is short and thus it is not difficult to estimate the scheduling delay. Also, this results in a waste of resources as it induces a lot of idle time during the execution, if the overhead is shorter than the estimation. Second, overheads do not simply work as an attachment to the job runtime and it involves a lot more complicated patterns

such as periodicity [18].

In this section, we first present our work on evaluating the overhead robustness of scheduling heuristics and we indicate a list of structural heuristics that are overhead robust. Second, since the estimate of overhead duration is difficult, we develop new heuristics that leverage the pattern information of workflow overheads, which represents a new approach to design overhead robust algorithms. To the best of our knowledge, so far, no study has systematically tried to evaluate the scheduling heuristics with respect to the overhead robustness.

### 6.1. Overhead Patterns

In this section, we introduce the common overhead patterns in workflow execution. In scientific workflow systems, time related functionalities such as workflow scheduling normally requires effective forecasting of activity patterns. In this work, we mainly focus on the overhead pattern that refers to a representative time series of overhead activities that occurs repeatedly and regularly in workflow execution. An overhead pattern is composed of ordered overhead activities obtained from scientific workflow system logs or other forms of historical data. Pattern discovery [41] usually starts from a periodical sampling plan to build representative duration series (Job Release, etc. ) and then conducts time-series segmentation to discover the pattern sets and predicts the activity duration intervals with pattern matching results.

The motivation for pattern based analysis comes from the observation that for those duration-series segments where the number of concurrent activity instances is similar, these activity durations reveal comparable statistical features. Due to the dynamic nature of underlying resources, pattern based forecasting of overheads can improve the effectiveness of scheduling heuristics.

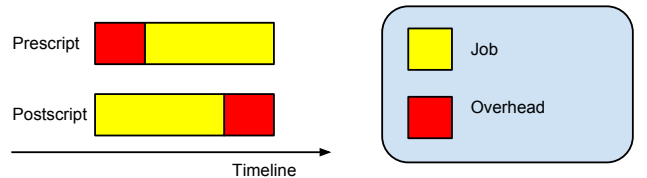


Figure 15: Adherence Pattern

Most of the work [24, 35] view the overhead duration as an attachment to runtime in workflow timeline. For example, the Pre/Post-script Delay is usually constant, which we call it Adherence Pattern as shown in Fig. 15. Scheduling algorithms can just add the delay to the job runtime without significant change to the algorithms. For this pattern, we have shown in our prior work [66] that it does not have much influence on the overhead robustness. However, we observe that the Workflow Engine Delay and the Queue Delay increases periodically and steadily. For example, Fig. 16 shows the Gantt chart of part of a real trace<sup>1</sup>. The Workflow Engine Delay (red) of the first

<sup>1</sup>Details: <http://www.isi.edu/~wchen/fgrid/run>

16 jobs is 5 seconds and then it increases to 10 seconds. We call this common overhead pattern the Incremental and Periodical Pattern (IPP). We observe the Queue Delay also increases periodically but the period is interrupted by the resource availability and thus it has a more complicated IPP. In the rest of this paper, we focus on the IPP of the Workflow Engine Delay and we will cover the Queue Delay in our future work. The reason why IPP prevalently exists is that many workflow management components are queue based systems. They repeatedly check their queues to find whether there are idle jobs, if yes they will process and submit these jobs, otherwise it will wait for a interval and continue. In Fig. 17 we abstract the IPP from the trace, which shows a repeatedly increase by a interval. We define throughput of a workflow management component as the maximum number of allowed jobs in queue. For example, the interval and the throughput of the Workflow Engine in Fig. 16 are around 5 seconds and 16 respectively.

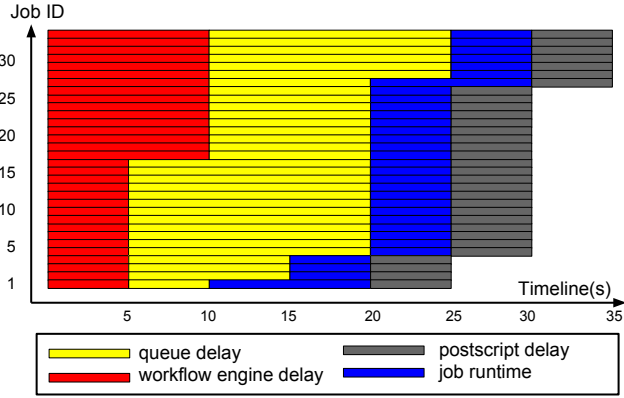


Figure 16: Workflow Execution Gantt Chart of a Real Trace

These overhead patterns reappear frequently during a duration series and they represent unique behavior of the workflow management components. After we define and discover these typical patterns, the intervals and throughputs of these patterns can be estimated and statistically captured from historical traces.

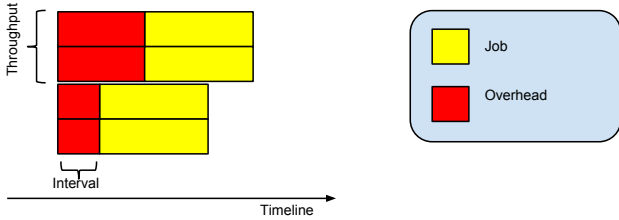


Figure 17: Incremental and Periodical Pattern

## 6.2. Overhead Robust Heuristics

In this section, we introduce the overhead robustness of four pairs of scheduling heuristics. Heuristics are widely used in

workflow scheduling since the scheduling problem is a NP-hard problem and the time complicity of a global optimization of the overall runtime is not affordable. Usually, heuristics utilize unique features of workflows or resources to guide the mapping of jobs to resources. For example, both of the MINMIN [33] algorithm and the MAXMIN [25] algorithm utilize the runtime of a job as the feature. However, they conduct the mapping in an opposite way, that is, MINMIN chooses the job with the shortest runtime while MAXMIN chooses the job with the longest runtime. Below we introduce the four pairs of scheduling heuristics including one that we propose.

**MINMIN and MAXMIN:** The MINMIN heuristic begins with a set of all unmapped jobs. Then, the set of minimum completion times for each job,  $M$  namely, is found. Next, the job with the overall minimum completion time from  $M$  is selected and assigned to the corresponding resource (hence the name MINMIN). Last, the newly mapped job is removed from the unmapped jobs, and the process repeats until all jobs are mapped. The MAXMIN heuristic is very similar to MINMIN. The MAXMIN heuristic also begins with the set of all unmapped jobs. Then, the set of minimum completion times,  $M$ , is found. Next, the job with the overall maximum completion time from  $M$  is selected and assigned to the corresponding resource (hence the name MAXMIN). Last, the newly mapped job is removed from the unmapped jobs, and the process repeats until all jobs are mapped. Intuitively speaking, we believe MAXMIN has better overhead robustness than MINMIN. As shown in Fig. 18, assuming we have two jobs and the interval of the overhead is 1. MAXMIN releases a job with longer runtime first, which can overlap with the increment of the overheads when MAXMIN releases the other job. However, the performance gain depends on the values of overhead interval, job runtime, overhead duration and the resource availability.

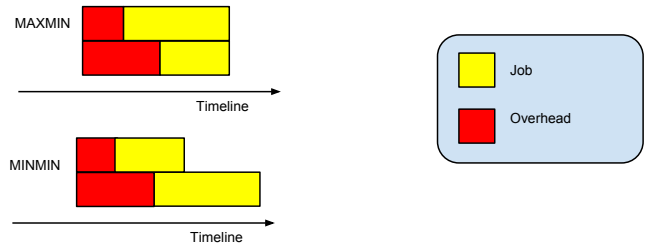


Figure 18: MAXMIN vs. MINMIN

**Breadth First and Depth First:** Namely, the Breadth First (BFS) algorithm iterates the jobs at the same workflow level (or depth within a workflow directed acyclic graph) first while the Depth First (DFS) algorithm iterates the jobs at the deepest workflow level first. Intuitively speaking, we believe BFS performs better than DFS in terms of overhead robustness since BFS releases more jobs at the same workflow level for most scientific workflows as shown in Fig. 20. Therefore, with enough jobs in queue, BFS can fully utilize the resources without wasting this overhead interval.

**Max Children First and Min Children First:** The Max Chil-

children First (MAXCH) algorithm sorts all the unmapped jobs based on the number of children jobs that they have and assigns the jobs with most children jobs first. The Min Children First (MINCH) algorithm works in the opposite way and assigns the jobs with least children jobs first. Similar to the case of BFS and DFS, we believe MAXCH should perform better than MINCH since MAXCH releases more jobs at the next level compared to MINCH and thus MAXCH can fully utilize the available resources.

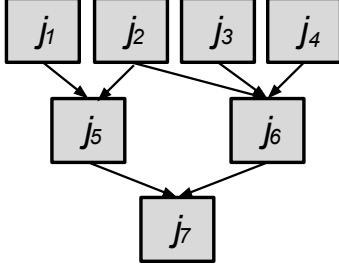


Figure 19: Impact Factor

*Important First and Unimportant First:* Here we propose a pair of Impact Factor based scheduling heuristics. The Important First (IFS) algorithm sorts all the unmapped jobs based on their *Impact Factor* (IF) and assigns the jobs with the largest IF first while the Unimportant First (UIFS) algorithm assigns the jobs with the smallest IF first. The **Impact Factor** (*IF*) of a job  $j_u$  is defined the same as Eq. 3. For simplicity, we assume the *IF* of a workflow exit job (e.g.  $j_7$  in Fig. 19) as 1.0. For instance, consider the workflow in Fig. 19. *IF* for  $j_1$ ,  $j_2$ ,  $j_3$ , and  $j_4$  are computed as follows:

$$\begin{aligned} IF(j_7) &= 1.0, IF(j_6) = IF(j_5) = IF(j_7)/2 = 0.5 \\ IF(j_1) &= IF(j_5)/2 = 0.25 \\ IF(j_2) &= IF(j_5)/2 + IF(j_6)/3 = 0.42 \\ IF(j_3) &= IF(j_4) = IF(j_6)/3 = 0.17 \end{aligned}$$

Thus, IFS algorithm should schedule  $j_2$  first while UIFS algorithm should schedule  $j_3$  or  $j_4$  first. The intuition of Impact Factor is that we aim to measure the relative importance of a job to the entire graph. Intuitively speaking, tasks with larger impact factors should have more impacts on the remaining jobs compared to tasks with smaller impact factors. For example, a bottleneck usually has a larger IF since it controls the release of more jobs. Similar to the case of MAXCH and MINCH, we believe IFS has a better overhead robustness than UIFS since IFS releases more jobs at the next few levels compared to UIFS.

Table 11 summarizes the heuristics and their potential overhead robustness.

Table 11: Scheduling Heuristics

Heuristics	Overhead Robust	Overhead Unrobust
Experiment 1	MAXMIN	MINMIN
Experiment 2	BFS	DFS
Experiment 3	MAXCH	MINCH
Experiment 4	IFS	UIFS

### 6.3. Experiment Conditions

The experiments presented hereafter evaluate the performance of the four pairs of heuristics mentioned ahead, which are widely used by workflow management systems.

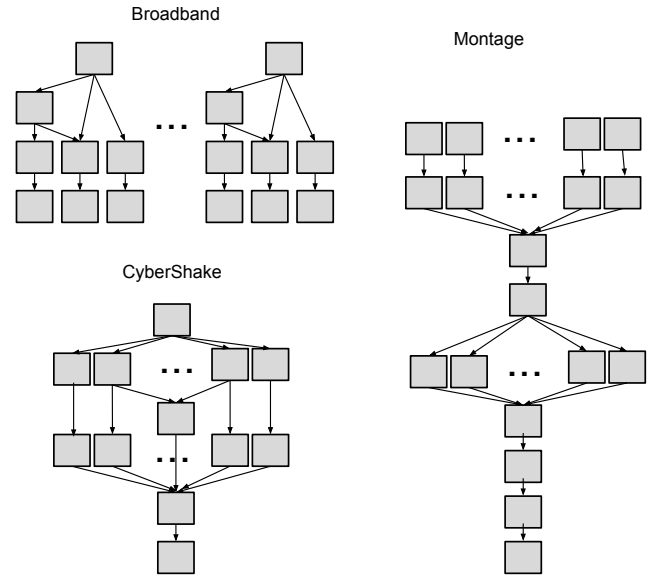


Figure 20: A simplified visualization of the Broadband workflow, the Montage workflow and the CyberShake workflow.

We extended the WorkflowSim [66] simulator with the overhead model to simulate a distributed environment where we could evaluate the overhead robustness of scheduling algorithms when varying the average overheads and throughput. As an initial attempt, we focus on the workflow engine delay ( $d$ ) in this paper. The simulated computing platform is composed by 20 single core virtual machines (worker nodes), which is the quota per user of some typical distributed environments such as Amazon EC2 [67] and FutureGrid [58]. Each machine has 512MB of memory and the capacity to process 1,000 million instructions per second.

Three workflows are used in the experiments: Broadband [73] is an application that enables researchers to combine long-period deterministic seismograms with high-frequency stochastic seismograms. Montage [3] is an astronomy application used to construct large image mosaics of the sky. CyberShake [74] is a seismology application that calculates Probabilistic Seismic Hazard curves for geographic sites in the South-



ern California region. All workflows are generated and varied using the WorkflowGenerator<sup>1</sup>. Each workflow instance is composed by around 100 tasks and its workflow structure is presented in Fig. 20. Runtime (average and task runtime distribution) and overhead (workflow engine delay and queue delay) information were collected from real traces production environments [18, 8], then used as input parameters for the simulations.

Four sets of experiments are conducted. Experiment 1 evaluates the relative robustness of MAXMIN and MINMIN by comparing the performance gain of the overhead robust heuristic (MAXMIN in this experiment) over the overhead unrobust heuristic (MINMIN), while varying the average interval of workflow engine ( $d$ ) and throughput of workflow engine ( $t$ ). Table 11 shows the heuristics compared in these experiments. Simulation results present a confidence level of 95%. Thus, for values of *Performance Gain* > 0, the overhead robust heuristics perform better than the respective overhead unrobust heuristics. Otherwise, the overhead robust heuristics perform poorer.

In these experiment sets, we vary the average throughput of workflow engine from 1 to 20 and we show the results of  $t=1, 5, 15, 20$ . The original throughput of workflow engine in these traces is 5 and a throughput that is larger than 20 does not influence the performance much since we have only 20 worker nodes in our experiments. We also vary the average interval of workflow engine from 0 to 100 seconds, which represents a typical range of workflow engine delay as shown in [18] and this range is able to show the difference of overhead robustness in these heuristics.

#### 6.4. Results and Discussion

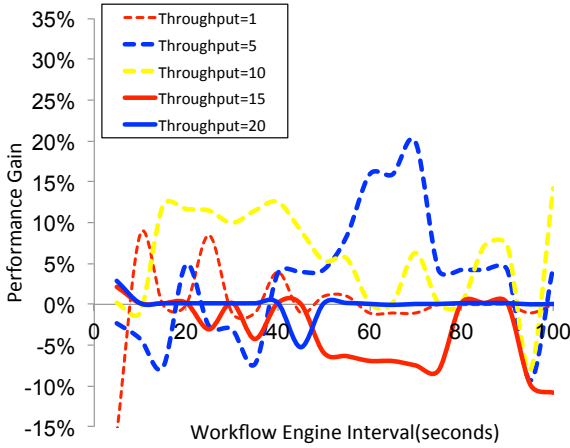


Figure 21: Broadband

Experiment 1: Fig. 21, 22, 23 show the *Performance Gain* of MAXMIN over MINMIN for the three workflows. We expected to see most *Performance Gain* > 0 if MAXMIN is a overhead robust heuristic compared to MINMIN. However, except for the Montage workflow, the *Performance Gain* is not significant for all of parameter settings, which concludes that

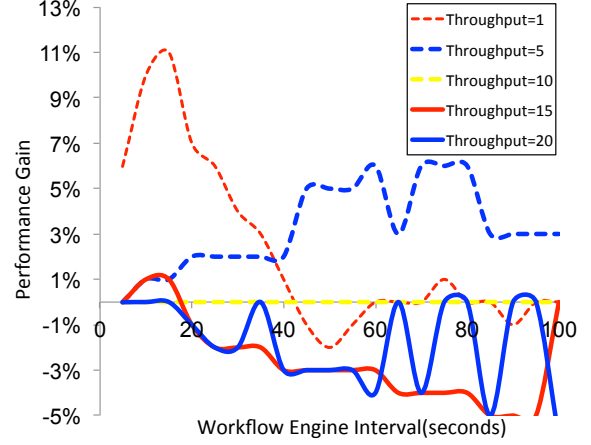


Figure 22: CyberShake

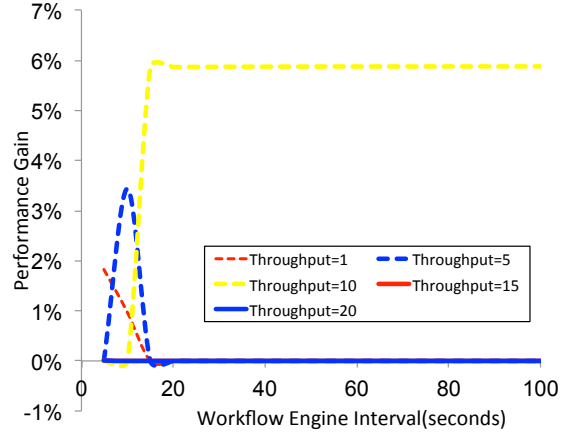


Figure 23: Montage

MAXMIN is not globally overwhelming MINMIN in terms of overhead robustness. The reason we believe is that the *Performance Gain* in this comparison highly depends on the ratio of job runtime, workflow engine delay, number of resources and throughput of workflow engine.

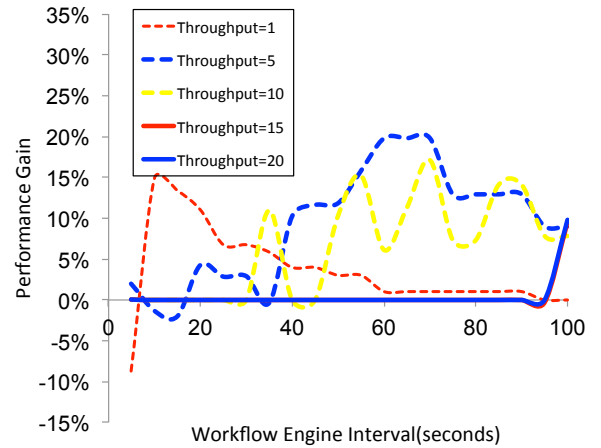


Figure 24: Broadband

<sup>1</sup><https://confluence.pegasus.isi.edu/display/pegasus/WorkflowGenerator>



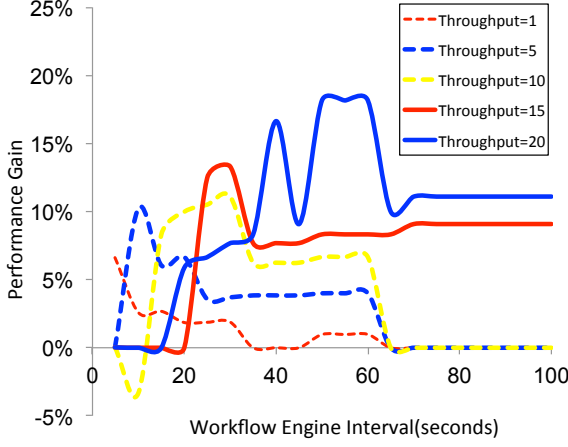


Figure 25: CyberShake

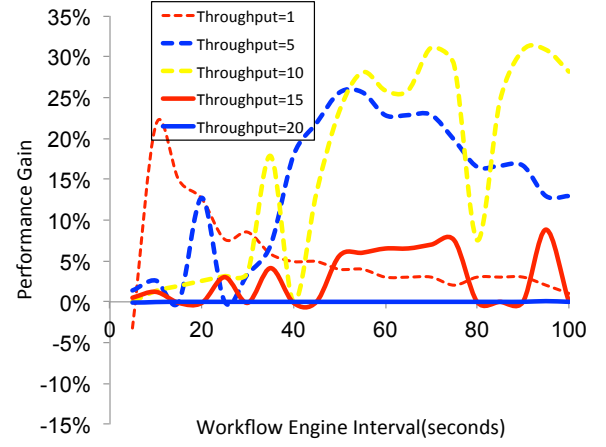


Figure 27: Broadband

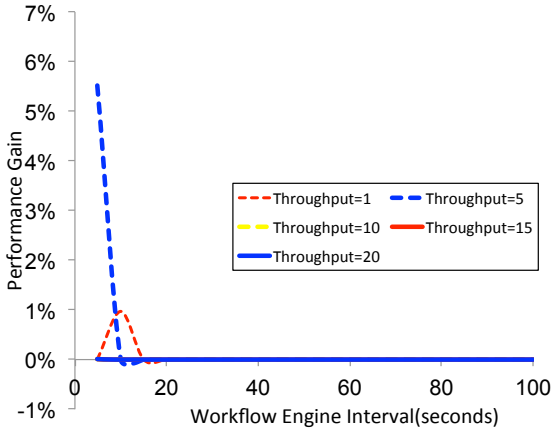


Figure 26: Montage

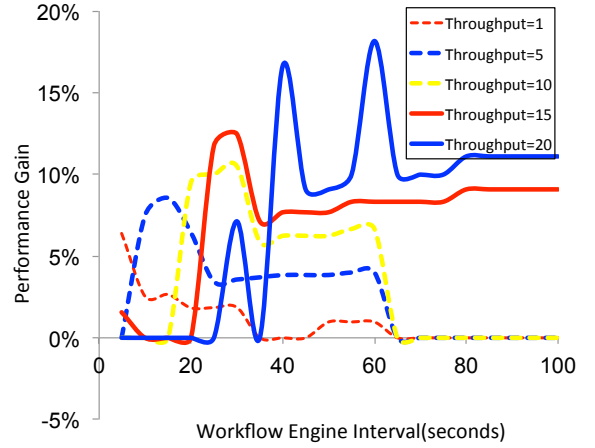


Figure 28: CyberShake

Experiment 2: Fig. 24, 25, 26 show the *Performance Gain* of BFS over DFS for the three workflows. We observe that most *Performance Gain*  $> 0$  and thus BFS performs better than DFS in terms of overhead robustness. What is more, Fig 25 shows with the increase of average throughput, the *Performance Gain* is more significant. We can also see that when the average throughput is high, the *Performance Gain* increases with the average interval of workflow engine. This suggests us in a real environment with a large overhead, we should use BFS instead of DFS.

Experiment 3: Fig. 27, 28, 29 show the *Performance Gain* of MAXCH over MINCH for the three workflows. We observe that most *Performance Gain*  $> 0$  and thus MAXCH performs better than MINCH in terms of overhead robustness, which is similar to Experiment 2. Comparing Fig. 24 and Fig. 27 we can see the *Performance Gain* of MAXCH over MINCH is more significant (30%) than that of BFS over DFS (20%).

Experiment 4: Fig. 30, 31, 32 show the *Performance Gain* of IFS over UIFS for the three workflows. We observe that most *Performance Gain*  $> 0$  and thus IFS performs better than UIFS in terms of overhead robustness, which is similar to Experiment 3. The reason is that for these workflows, IF based heuristics can produce similar schedule as the heuristics based

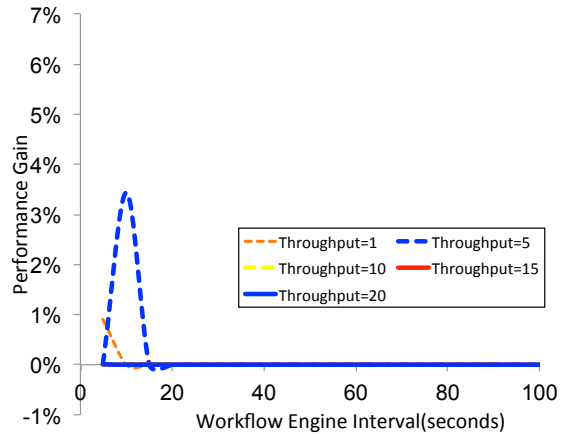


Figure 29: Montage

on the number of children. Most of the workflows used in this paper is not irregular enough and thus we are not able to show the difference of IF based heuristics and the heuristics based on the number of children.

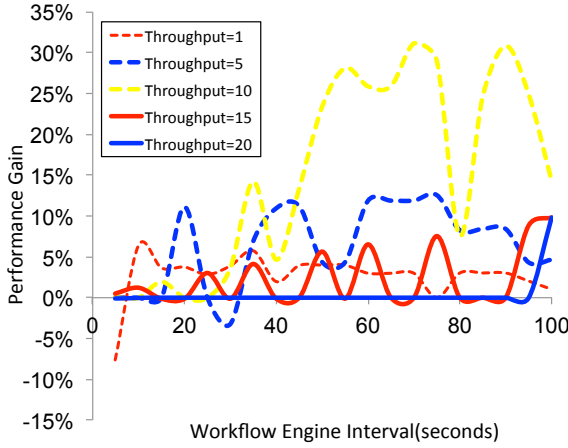


Figure 30: Broadband

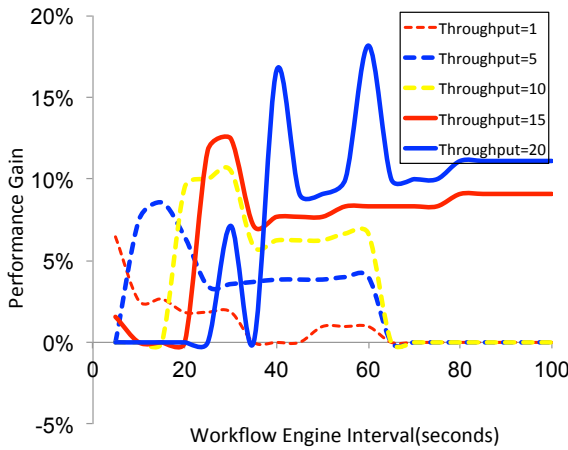


Figure 31: CyberShake

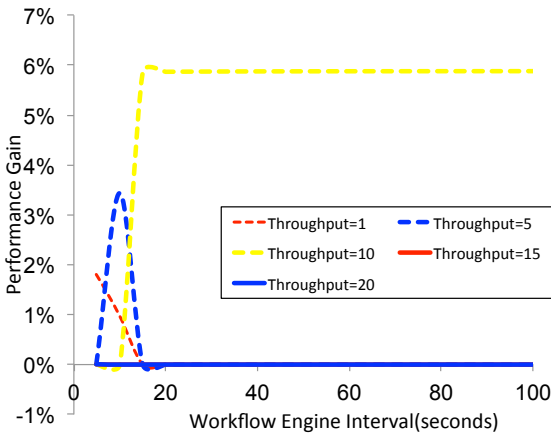


Figure 32: Montage

## 7. Conclusion, Discussion and Future Work

In this work, we introduced a series of quantitative and structural metrics in revealing workflow structure information and we further applied them to three usage scenario to show their influence with traced based analysis and simulations. The ex-

periments show that these metrics can significantly improve the performance of task clustering strategies and task scheduling strategies.

In our work, we have shown that these metrics have strong connection with the performance of different optimization methods. However, not all of them perform well under all of the circumstances. Also, the origin of these metrics are heavily depending on human intuition. Still, there is a lack of understanding of whether we can have more and better metrics in revealing how workflow structures interact with different optimization methods. As an initial effort, we will continue to use pattern discovery techniques to collect as many metrics as possible and performance experiments on them.

With enough metrics, one important step we are going to take is to aggregate multiple metrics and use machine learning techniques to reveal their correlation. However, combining the metrics we have proposed above is challenging. First, these metrics are quantitative and can be measured, however, on their own they are hard to compare against each other and determine whether one metric is more significant than others. Second, having multiple metrics together increase the complexity and this is against our initial goal, which is reduce the complexity in analyzing workflows. A more sophisticated alternative, however, is to conduct a statistical analysis based on Principal Component Analysis (PCA). This method determines in a more precise way the existing correlation between the collected metrics and their impact on workflow performance.

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