Abstract—When in need for executing complex sets of interrelated calculations on High-Performance Computing (HPC) environments the obvious choice is to use scientific workflows. As workload management software do not support the execution of interrelated tasks, workflow management systems have been introduced to execute workflows on HPC environments. Recently, a new distributed architectural model that offers dynamic workflow execution capabilities to workflow management systems is introduced. It executes workflows on a per-task basis. While this approach facilitates dynamic workflows, it adds a considerable overhead to workflows substantially increasing their makespans. As most workflows are static, task-wise execution of workflows degrades the performance of most workflows. In this paper, we introduce a distributed workflow management system, SwarmForm that introduces task clustering to the new architectural model.

SwarmForm is open source and offers better performance than existing distributed workflow management systems by clustering workflow tasks to reduce overheads while allowing the users to choose between task-wise and cluster-wise execution of workflows depending on the workflow nature. The paper proves that SwarmForm enables the use of all the features introduced with the new architectural model while providing better makespans for scientific workflows.

Keywords—Task Clustering, Workflow Management Systems, Scientific Workflows.

I. INTRODUCTION

Almost every scientific domain such as Astrophysics, Bio and health informatics, Physics, and Bio-Sciences use workflows to express complex sets of tasks that are dependent on one another using Scientific workflows. These workflows are executed in High-Performance Computing (HPC) environments as they need a lot of computing power to execute. Workload management software like PBS Pro [1], SLURM [2], TORQUE [3] are installed on these HPC environments to manage the computing resources of the environment. However, they do not support workflow scheduling but only support the execution of independent jobs.

Given the complexity of real-world workflows, the execution becomes cumbersome as the users have to manage a large number of individual job execution files. Therefore, Workflow Management Systems (WMS) have been introduced to execute scientific workflows on HPC environments.

A workflow management system is able to get a workflow consisting of a series of interrelated tasks as input and submit them as separate jobs to a workload management software while maintaining the dependencies between the tasks in order to be executed in an HPC environment. WMSs execute workflows either by executing each task as a job and passing its results to other tasks (Chained Jobs) or by executing the whole workflow as a single job (Pilot Job). Running a workflow as a pilot job results in better makespan with poor resource utilization of the execution environment whereas running a workflow as chained jobs results in better resource utilization with poor makespan.

Distributed WMSs execute workflows as chained jobs with a separate job for each task whereas centralized WMSs execute workflows as pilot jobs. Therefore, centralized WMSs have better makespan with poor resource utilization while distributed WMSs have better resource utilization with poor makespan. Although centralized WMSs minimize this issue by clustering the tasks in the workflow and submitting them as few chained jobs, they fail to provide many features available in distributed WMSs like dynamic workflows, concurrent execution of multiple workflows, failure detection and correction, etc. Therefore, it is observed that distributed WMSs offer much more important functions than centralized WMSs.

Scheduling a job on an HPC environment consists of a considerable overhead [4]. Thus, scheduling of jobs using a distributed WMS causes a significant increase in the makespan of the workflow as they execute each task as a separate job. The advantages offered by distributed WMSs can be retained while reducing the makespan of workflows by introducing task clustering to distributed WMSs. This is clearly demonstrated in Fig. 1(a) where the jobs are scheduled in the chained fashion resulting in a longer makespan and Fig. 1(b) where the jobs are executed within a much shorter makespan with somewhat of a compromise on the resource utilization. However, there is a significant potential to improve the resource utilization while...
having pilot jobs in a chained fashion to make a near optimal balance of trades.

Fig. 1(a) Running a workflow as a set of Chained jobs

Fig. 1(b) Running a workflow as a Pilot job

The paper presents the following contributions to the domain of workflow scheduling:

- The research introduces SwarmForm [5] a new open source distributed workflow management system with task clustering capabilities.
- The research introduces an extension to the existing Workflow and Platform Aware Clustering algorithm [6] to improve its performance
- The research implements the Resource Aware Clustering (RAC) algorithm [7] in SwarmForm to maximize the resource utilization of the clustered workflows that are executed through SwarmForm

The rest of the paper is arranged as follows. Section II presents a review of the existing literature and background of the study. Section III presents the work proposed in the study. Section IV evaluates the performance improvement introduced by the proposed work and Section V concludes the paper with an overview on the future work in Section VI.

II. RELATED WORK

Liu et al. [8] show that the functional architecture of a WMS consists of 5 layers - Workflow Execution Plan (WEP) generation, WEP execution, Presentation, User services, and Infrastructure. According to how these layers are managed, existing WMSs can be categorized as centralized WMSs and distributed WMSs. In WMSs like Pegasus [9], Taverna [10], Kepler [13] have been used for over a decade for executing workflows in many high-performance computing environments all around the world. They include features such as workflow submission, special CLI tools for workflow design and management, ability to store provenance data, etc.

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These systems are much more effective in executing scientific workflows than using workload management software for scientific workflow execution. The inability to execute dynamic workflows can be seen as the major drawback of the centralized WMSs. All these systems need the workflows to be defined at the beginning of the workflow and they do not allow modifying the workflow while it is being executed. In addition to that, most of them run workflows as a single pilot job. As explained by Rodrigo et al. [14] executing a workflow as a single pilot job causes a huge resource wastage as many of the resources of the HPC environment are idle most of the time. Furthermore, they do not support concurrent execution of workflows as they are submitted as pilot jobs.

The above issues have been addressed in eHive [11] and FireWorks [12] using a new architectural model. They follow a blackboard-based architecture with 3 main components: a central database that holds details of each workflow submitted by the users, a set of clients that pull tasks from the database and execute them on the backend and a client manager that handles spawning, killing, and managing of the clients.

The distributed architecture resolves the single point of failure in the existing centralized systems by having different programs control different layers in workflow management. In addition to that, these systems support concurrent execution of multiple workflows and the system manages the scheduling of tasks across workflows. Distributed WMSs submit workflows as chained jobs with each task packed as a single job. This allows the workflows to change its structure at the runtime while resulting in a substantial increase in resource utilization of the execution environment as only the required resources are obtained per each job. It also makes sure that the failure of one job does not affect the execution of other jobs.

Three major overheads are present when executing a job on an HPC environment: i.e., Scheduling overhead (Time taken to schedule the job on a specific node), Queue Delay (Time a job must wait in the queue until it gets the opportunity to be executed) and Communication Overhead (Time taken to transfer the results of parent job to its children). Therefore,
executing each task of a workflow as separately chained jobs will cause a substantial increase in the makespan \([14]\) as executing each job adds a considerable overhead to the total runtime of the workflow.

While distributed WMSs offer a lot of features that are not available in centralized WMSs, the increased makespan of workflows due to the execution of each task as a chained job raises a major concern. Even though this adds support for dynamic workflows, executing both static and dynamic workflows as individually chained jobs cause an unnecessary overhead. A better approach to this problem would be to introduce task clustering to distributed WMSs and allow the user to decide whether he needs clustering or not depending upon the application. This will reduce the makespan of workflows in distributed WMSs while ensuring that all the advantages offered by distributed WMSs are preserved.

To address this issue, we introduce a new distributed workflow management system SwarmForm which includes task clustering to reduce the makespan of workflows. Using SwarmForm, we intend to deliver all the advantages of a distributed WMS to users while maintaining the optimum balance between the makespan of workflows and the resource utilization of the environments.

Task clustering is already implemented in some of the centralized WMSs like Pegasus \([9]\) and in some Grid middleware management systems like Xavantes \([15]\); we intend to use those techniques to provide better makespans for workflows executed using distributed WMSs.

Different researches have introduced different clustering techniques. In the related literature, Horizontal Runtime Balancing, Horizontal Impact Factor Balancing and Horizontal Distance Balancing algorithms introduced by Chen et al. \([16]\) are being used as the baseline for workflow task clustering. Kaur et al. \([17]\) has introduced a new clustering technique called Hybrid Balanced Task Clustering Algorithm that clusters tasks both vertically and horizontally. Chen et al. \([16]\) has introduced a Balanced clustering technique for horizontal clustering and Sahni et al. \([6]\) has introduced the Workflow and Platform Aware task clustering (WPA) Algorithm. Zhang et al. \([18]\) has introduced a new metric called Dependency Correlation to cluster tasks in their Dependency Balance Clustering Algorithm. Under the proposed technique, first, the tasks with single-child single-parent relationships are clustered together and then the resulting tasks are clustered horizontally using the WPA algorithm. The WPA algorithm takes the available number of computing nodes as an input. Since in most of the HPC environments we cannot get the exact number of resources available at the time of execution, we have proposed a slight modification to the WPA algorithm along with the addition of our vertical clustering approach. The modified pseudocode of the WPA algorithm is given in algorithm 1.

### Algorithm 1: Extended Workflow-and-platform aware clustering algorithm

1. procedure **WPA**\([\text{Workflow } w] \)
2. Begin
3. \( w \leftarrow \text{ClusterSingleParentSingleChild}(w) \)
4. for level = depth\([w]\) to 2 step -1 do
5. \( cLateness \leftarrow \{\} \)
6. taskList \leftarrow getTasksAtLevel\([w, \text{level}] \)
7. taskList \leftarrow SortTasksByIncreasingOrderOfTheLongestParent\([\text{taskList}] \)
8. for each task \( t \) in taskList do
9. \( cLateness \leftarrow \text{AssignParentsToClusters}(t) \)
10. Add \( cLateness \) to \( cLateness \)
11. end for
12. taskListParents \leftarrow getParents\([\text{taskList}] \)
13. \( w \leftarrow w - \text{taskListParents} \)
14. end for
15. end procedure

Under the proposed technique, first, the tasks with single-child single-parent relationships are clustered together and then the resulting tasks are clustered horizontally using the WPA algorithm. The WPA algorithm takes the available number of computing nodes as an input. Since in most of the HPC environments we cannot get the exact number of resources available at the time of execution, we have proposed a slight modification to the WPA algorithm along with the addition of our vertical clustering approach. The modified pseudocode of the WPA algorithm is given in algorithm 1.
Fig. 2 illustrates the significance of this task clustering approach. Fig. 2(a) depicts an example workflow with 5 levels and the number on each node states the execution time of the task. First, the tasks are being clustered vertically considering their single-parent single-child relationships (Fig. 2(b)). Fig. 2(c) shows the result of the proposed vertical clustering technique on the example workflow of Fig. 2(a). Then the resulting workflow tasks are clustered horizontally using the WPA algorithm (Fig. 2(e)). Fig. 2(d) shows the result of our proposed extended WPA clustering algorithm.

The algorithm 2 explains the pseudocode of the proposed vertical clustering technique. The algorithm takes a workflow as the input. It begins with the first level of the workflow and iterates to the depth of the workflow (Line 3). It selects the tasks at each level (Line 4) and iterates the tasks, one by one (Line 5). If the task only has a single child and that child task has no other parents (single-parent single-child relationship), both the task and its child task are grouped into a cluster. This process is repeated in a depth-first manner until there are no more single-parent single-child relationships for the selected task (Line 7-10). Finally, the workflow is updated if a selected task is clustered with its children (Line 13).

B. SwarmForm Workflow Management System

1) SwarmForm Architecture: SwarmForm distributed WMS is developed on top of FireWorks [12] distributed WMS which is the state-of-the-art system in the domain of distributed WMSs. FireWorks is used as an open source library in the implementation of SwarmForm. SwarmForm ensures that all the functionalities of FireWorks are available to the user while offering additional functionalities for workflow management. SwarmForm is highly decoupled from FireWorks and this approach provides the ability to develop FireWorks and SwarmForm independently ensuring fast and easy adaptations to any update to FireWorks.

The architecture of SwarmForm bears a close resemblance to FireWorks with some additional improvements. In SwarmForm, a workflow is referred to as a SwarmFlow. A SwarmFlow can be represented as a Directly Acyclic Graph (DAG) and these SwarmFlows can be defined by the Python interface, command-line interface or by directly loading a JSON or YAML SwarmFlow definition. SwarmForm adapts the workflow definition format introduced by FireWorks for defining SwarmFlows as this format helps to define workflows in a more easy and readable way in contrast to the existing DAX format.

A SwarmFlow consists of one or more individual tasks that are called Fireworks (FWs). These FWs represent the nodes in the SwarmFlow definition DAG whereas the edges of the DAG represent dependencies between FWs. A Firework can have a sequence of one or more atomic tasks that are called FireTasks. These FireTasks are separate Python functions that can call shell scripts, transfer files, read/write files or call other Python functions. FireTasks can return FWActions that can modify the SwarmFlow dynamically at runtime based on the computational conditions which give the dynamic behaviour to the system. SwarmPad is another key part of the SwarmForm WMS that is used to store all the details of SwarmFlows, FWs, provenance data and other data related to execution of SwarmFlows. SwarmPad is a NoSQL database which is built using MongoDB. FireWorkers are the clients who pull FWs from the SwarmPad and execute. It launches unique agents called Rockets to pull and execute each FW. Workflow management is handled by the SwarmPad and workflow execution is handled by Rockets and FireWorkers which provides the distributed behaviour to the SwarmForm WMS.

Fig. 3 shows the architecture of the SwarmForm WMS. The FlowParser takes the input workflow and passes it to the SwarmFormer. SwarmFormer clusters the SwarmFlow and adds it to the database. Optionally, the FlowParser can save the SwarmFlows directly to the database without clustering, based on the user requirement. The SwarmFormer takes a SwarmFlow as the input and clusters the tasks in the SwarmFlow and saves the clustered SwarmFlow in the database. Later, the FireWorkers can pull tasks using Rockets and execute clustered Fireworks in HPC environments as shown in Fig. 3.
2) SwarmForm Features: As we have described above, the overhead in executing a job is a critical factor which results in increasing the makespan of a workflow. Even the state-of-the-art distributed workflow management system does not address this issue as it executes each task in a workflow as a separately chained job. As a solution to the aforementioned problem, we introduce task clustering to SwarmForm which reduces the makespan of the workflows by minimizing the overheads in the execution of a workflow. In section IV, we have proven that SwarmForm outperforms the state-of-the-art distributed WMS FireWorks [12] when task clustering is enabled.

In SwarmForm, workflows which are referred to as SwarmFlows are treated as primary entities and Fireworks are considered as secondary entities. This considerably eases the process of managing workflows when executing workflow operations like task clustering. In addition to that, SwarmFlow can accept and process multiple task parameters like cost, execution time, resource requirements of the task etc. These parameters can be used for making better scheduling decisions and workflow management decisions like how the tasks will be clustered which increases the performance of the system.

The support to these parameters is added in such a way that a user can easily extend the parameter set by easily adding new parameters. The WMS takes cost parameters like execution time, required number of cores per task as inputs through _queueadapter identifier in the workflow definition. Therefore, users will be able to define new parameters like memory required, wall time etc. which can be used in further workflow management decisions.

Initially, SwarmForm was only equipped with the WPA clustering algorithm, which did not consider the resource requirements when making task clustering decisions. Later, we implemented the RAC algorithm [7] which takes both execution time and resource requirements into consideration when making task clustering decisions. Although the RAC algorithm does not always outperform the existing task clustering algorithms in makespan reduction of workflows, it outperforms all the existing task clustering algorithms in maximizing resource utilization while providing competitive makespan reductions in workflows. Therefore, RAC algorithm [7] is implemented in SwarmForm to maximize the resource utilization of the execution environment while minimizing the makespan of the workflow.

Since the scientific workflow is represented as a directed acyclic graph (DAG), we have defined our data structure to model the workflow in SwarmForm which we referred to as DAG model. That DAG model is used to implement the WPA algorithm. The same approach is followed when implementing...
the RAC algorithm. The algorithm takes the workflow represented using the DAG object and number of clusters per horizontal level (R) as the inputs and returns a DAG object which represents the workflow with clustered tasks. The algorithm traverses the DAG following a level-by-level approach, starting from level one. It takes the tasks at each level and clusters the tasks at level only if the number of tasks at level is greater than the number of clusters per level. In each level, first it creates R number of empty clusters and iterates the tasks in the level task by task. In each iteration in the inner loop the resource aware clustering factor is calculated for the task respective to the clusters created for that level. Then it selects the cluster with the minimum factor value since resource-aware clustering factor gives the smallest value with the cluster that the considering task fits best and checks whether the cluster has not exceeded the number of tasks that it can hold. If it does not exceed, the task is put into that cluster. This process is repeated for each task in each level. After populating the clusters by tasks for each layer workflow DAG is updated as it needs to preserve the dependencies. First, it removes the task in the considering level from the workflow DAG and adds the new clusters to the workflow. Then updates the parent-child relationships appropriately as the updated workflow DAG needs to preserve the dependencies between tasks.

IV. RESULTS

In this section, we evaluate the performance of SwarmForm WMS. As FireWorks is the state-of-the-art in distributed workflow management systems, WPA task clustering enabled SwarmForm WMS is compared and evaluated against the FireWorks WMS. To have the same evaluation setup for both systems, we have evaluated both WMSs on standard benchmark workflows CyberShake (Fig. 4), LIGO (Fig. 5) and SIPHT (Fig. 6) presented by Bharathi et al. [19].

The workflow definitions of CyberShake 100 job workflow, LIGO 100 job workflow, and SIPHT 97 job workflow provided by Pegasus workflow generator are used for the evaluation [20]. We use a workflow simulation setup for evaluating the performance of the systems. This is a widely used approach since reserving an HPC environment for evaluation purposes is highly costly. The simulation setup consists of 5 rockets with each rocket acting as a computing node with a single core. Each rocket pulls a job from the database and executes it. We have added a constant delay after completion of each job to represent the communication overhead incurred when transferring the output of a parent job to its children jobs. Only the considered workflow is present in the database throughout the evaluation.

Initially, two sets of the same workflows in DAX format are taken and converted into SwarmForm/Firework readable format using the SwarmForm workflow generator. Then, a set of workflows are clustered and executed using the SwarmForm WMS and the other set of workflows are directly executed using the FireWorks WMS. Makespan of each workflow is measured in both systems and the Performance Gain (3) is calculated.

\[
\text{Performance Gain} = \frac{\text{Makespan of executing the workflow in FireWorks}}{\text{Makespan of executing the workflow in SwarmForm}} - 1
\]

From Fig. 7, it can be observed that the makespan of each workflow has been reduced when executed using SwarmForm than with FireWorks. This proves that executing workflows with task clustering enabled in SwarmForm reduces the makespan of each workflow considerably than executing it in FireWorks.
The Performance Gain shows the percentage improvement in the makespan of each workflow executed in SwarmForm compared to FireWorks. From the results of the experiments, it can be observed that SwarmForm shows a 10.19% improvement in the makespan of CyberShake, 24.36% improvement in the makespan of LIGO and 9.41% improvement in the makespan of SIPHT workflows. Further, it should be noted that the performance gain of each workflow is positive which shows that SwarmForm outperforms FireWorks when task clustering is enabled.

In this evaluation, we have considered only the communication delay between tasks and the queue delay among jobs in the same workflow as the overhead. Clustering related tasks together eliminate the communication overhead between those tasks as they are executed in the same node under the same job. The improvement shown in the evaluation mainly results from the reduction of communication overhead between the tasks. However, in real environments, there are many more overheads like scheduling overhead and queue delays due to the competition for limited resources by a large number of jobs from multiple workflows. Among them, queue delay can increase the makespan by a substantial amount as the delay increases considerably with the increase of the job submissions. These overheads are reduced when tasks are clustered. Therefore, we expect that SwarmForm will perform even better when used with real workflows in HPC environments.

V. DISCUSSIONS

This paper presents SwarmForm, a new distributed workflow management system with task clustering capabilities. SwarmForm is built using FireWorks which is an open source library and offers useful features such as support for dynamic workflows, concurrent workflow execution, and failure detection and correction that are not available in the existing centralized WMSs. SwarmForm introduces task clustering to increase the performance of existing distributed WMSs, a DAX workflow importer and a workflow generator that can be used for workflow simulation purposes.

As another contribution, the research has introduced an extension to the WPA algorithm which improves its performance. The extension of the WPA algorithm is to introduce a hybrid clustering approach, which clusters the tasks both vertically and horizontally. We implement the updated clustering algorithm in SwarmForm and evaluate SwarmForm with FireWorks and prove that execution of workflows in SwarmForm yields better makespans than executing them in the existing state-of-the-art distributed WMS due to the introduction of task clustering.

Finally, we implement the RAC algorithm as the primary clustering algorithm in SwarmForm to introduce resource management capabilities to SwarmForm. None of the existing WMSs consider minimizing resource wastage when clustering tasks. Therefore, executing workflows using SwarmForm by clustering their tasks with RAC algorithm significantly reduces the resource wastage of the execution environment while providing a considerable improvement in the makespan of the workflow. Further, the users are given the opportunity to choose any of the task clustering algorithms depending on the requirement for clustering their workflows while providing the developers with the ability to implement any required task clustering algorithm and use them without having to change any core components of SwarmForm. The estimated resource wastage after clustering of workflows with each clustering algorithm is also shown to the users which allows them to choose the algorithm that gives them the best resource utilization and the makespan.

VI. FUTURE WORK

Task clustering is done to achieve different objectives along with reducing makespan like minimizing resource wastage, minimizing dependency imbalance, achieving QoS requirements etc. Currently, SwarmForm contains only two task clustering algorithms which are capable of solving resource imbalance and runtime imbalance problems. We plan to implement a few more task clustering algorithms in SwarmForm thus allowing the user to choose the suitable one.
algorithm depending on the use case from a variety of task clustering algorithms.

We plan to improve our workflow generator to generate actual workflows and to import actual workflows defined in DAX format into SwarmForm workflow definition format. It will later be extended to support Common Workflow Language [21] as well. Further, we plan to introduce a GUI to SwarmForm to easily define new workflows graphically as the existing distributed WMSs consist of Graphical User Interfaces (GUI) only for reporting.

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