Efficient Runtime Environment for Coupled Multi-Physics Simulations: Dynamic Resource Allocation and Load-Balancing

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Abstract

Coupled Multi-Physics simulations, such as hybrid CFD-MD simulations, represent an increasingly important class of scientific applications. Often the physical problems of interest demand the use of high-end computers, such as TeraGrid resources, which are often accessible only via batch-queues. Batch-queue systems are not developed to natively support the coordinated scheduling of jobs – which in turn is required to support the concurrent execution required by coupled multi-physics simulations. In this paper we develop and demonstrate a novel approach to overcome the lack of native support for coordinated job submission requirement associated with coupled runs. We establish the performance advantages arising from our solution, which is a generalization of the Pilot-Job concept – which in of itself is not new, but is being applied to coupled simulations for the first time. Our solution not only overcomes the initial co-scheduling problem, but also provides a dynamic resource allocation mechanism. Support for such dynamic resources is critical for a load-balancing mechanism, which we develop and demonstrate to be effective at reducing the total time-to-solution of the problem. We establish that the performance advantage of using BigJobs is invariant with the size of the machine as well as the size of the physical model under investigation. The Pilot-Job abstraction is developed using SAGA, which provides an infrastructure agnostic implementation, and which can seamlessly execute and utilize distributed resources.

I. Introduction

Coupled Multi-Physics simulation techniques are being increasingly used to study many different physical phenomena spanning time and length scales at different levels of detail [1] [2]. These techniques have been used to investigate phenomena from crack-propagation in materials, biological systems as well as understanding multi-phase fluid flow in constrained geometry.

In addition to the "physics challenges" of these Multi-Physics coupled simulations, there exist interesting "computational challenges". Probably the best known (and investigated) is the challenge of simulating large and complex systems, leading to simulations that require greater computational resources – often involving HPC resources. Parallelization helps individual codes address the computational demand of large and complex systems, but incorporating two distinct codes under the umbrella of a single tightly-coupled application (say using MPI) is not without significant problems. For example, the two codes can often have very different computational kernels (one could be mesh-based, the other unstructured particle simulations) with very different computational time-scales.

Here we will focus on the challenges arising from running tightly-coupled simulations on production systems with batch-queues, whereby it cannot be guaranteed that two separate jobs will execute concurrently. Specifically we will consider the case of coupling a Computational Fluid Dynamics (CFD) code and a Molecular Dynamics (MD) code, where the communication is via the exchange of files and not Unix pipes (see next section for details on the coupling).

Although not exactly tightly-coupled in the sense of MPI, viz., very frequent and with an extreme sensitivity to latency in communication delay, the CFD and MD codes communicate frequently, (e.g., the CFD code conducts data exchange in every iteration) and thus they need to run concurrently. Thus, without explicit support for co-scheduling, it is unlikely that coupled CFD-MD simulations will run concurrently as inevitably the first job to run will have to wait for the other to follow.

Another important challenge, especially for large-scale simulations is the need for efficient load-balancing, taking into account the individual application's performance. Even if the two simulations could run concurrently, without explicit load-management/balancing support, there is likely to be inefficient utilization of compute resources due to load imbalance. As the performance of each simulation component changes with computing resource and problem size, re-adjustment of allocated resources to each task according to their performance is required during the simulation. Interestingly, as we will show, effective load-balancing of two independent but concurrently running codes introduces the need for dynamic resource allocation, and the same solution that we devise to overcome the concurrent scheduling requirement/constraints of coupled jobs also supports the feature of dynamic resource allocation. In contrast, if simulations were submitted as independent jobs, changing resource (CPU) allocation to address these changes is challenging – as the change in resource assigned to one is correlated with a change in resource assigned to the other component.

The Pilot-Job is just a container task where a number of sub-tasks can run in a pre-defined schedule with the specified number of processors whether or not they are coupled. The dynamic resource allocation capabilities of the Pilot-Job prove useful in our scenario of using multiple Pilot-Jobs on the single container task as well as when using load-balancing in the single-resource scenario. Although the container-Job/Pilot-Job concept is not novel *per se*, we believe this is the first documented utilization of these abstractions to perform coupled Multi-Physics simulations. We claim that there several distinct advantages that arise as a consequence of using Pilot-Jobs for Coupled Simulations: (i) obviates the need for a co-scheduler while preserving performance, (ii) enables dynamic resource allocation, which in turn is important for load-balancing across coupled simulations. But given the lack of system or service-level support to address the challenges outlined above, there is a need to address the solution at the application level. This paper aims to provide novel solutions to the above problem using frameworks that are in user (application) space.

We will provide details on how we implement our solution in Section 3, but in a nutshell it is critical to mention that our solution and its concomitant efficiency is not tied to either a specific application set (or infrastructure) and is scalable and extensible. It is based on SAGA (the Simple API for Grid Applications) [3], which is a high-level API which provides the basic functionality required to implement distributed functionally – both logically and physically, in an infrastructure and middleware independent fashion. SAGA enables creation of higher levels of abstraction, such as a container-job or a Pilot-Job (which,

as we will discuss, is referred to as the BigJob [4]). The SAGA-based Pilot-Job is infrastructure neutral, unlike *all* other Pilot-Jobs.

We begin the next section with an outline of the basic motivation for coupled simulations and load balancing. We will address this fundamental question: Does the use of an infrastructure independent container job assist in the time to solution of a coupled simulation? We will determine that the answer is yes for a variety of different resource utilization scenarios. In the simplest case of a coupled simulation running on a single machine, we will establish that the reason is the lowered waiting time typically associated with a larger size request (on most queuing systems, for most commonly occurring load-factors). As our experiments will show, performance improvement arise from removing the need for scheduling the two-components separately and in providing a single job-requirement to the queuing system.

II. Hybrid CFD-MD Approach: Understanding the Coupling, Communication and Load-Balancing Requirements

The hybrid CFD/MD approach [5], [6], [7] is a simulation method which adopts the continuum hypothesis in capturing macroscopic features of a flow-field and details atomistic intermolecular interactions on interfaces of different materials by using the MD approach. CFD can accurately predict flow properties on conventional moderate/large size fluid domains, but is intrinsically impossible to reflect characteristics of surrounding solid materials. While MD can provide atomistic level resolution of interactions between particles, it becomes computationally demanding as the size of simulated system grows. So, neither method is suitable for solving a mesh-scale fluid system where the viscous effect dominates the flow characteristics but macroscopic features are also worth capturing efficiently. The best solution would be, as can be seen in Fig. 1, to carry out the hybrid CFD/MD approach with which atomistic interactions between solid elements and fluid particles near the wall is simulated by MD and the far field flow is calculated by CFD.

In this study, we built on the MPI version of the "in-house" incompressible CFD code [8] and the MPI version of LAMMPS [9] for MD. We did some modifications to these application codes to implement hybrid schemes on each application domain. In brief, the hybrid region where the coupling mechanism between MD region and CFD region is executed comprises five sub-regions. In the CFD boundary grid region positioned near the pure MD region, velocities of particles obtained with MD are averaged and used for boundary condition for the corresponding CFD computational cells. The MD boundary zone is placed above the CFD boundary zone and here the information
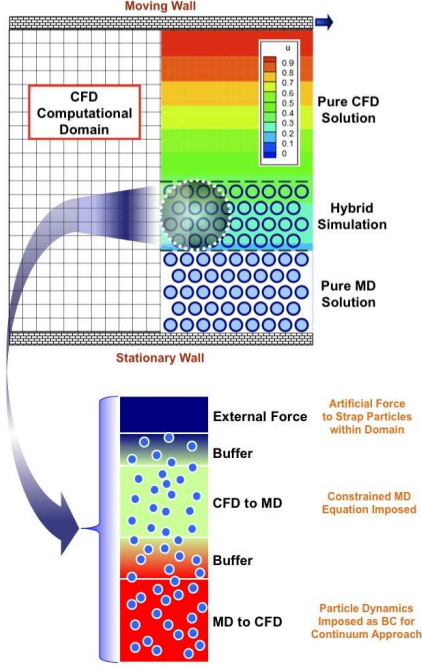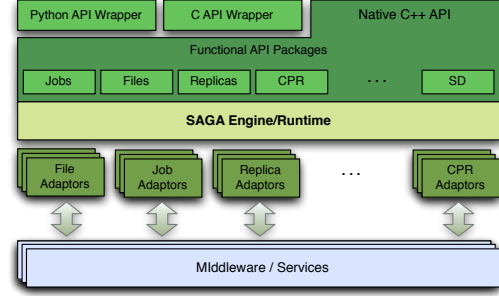
Fig. 1. Schematic of CFD/MD Coupled Simulation of Channel Flow and the velocity profiles at different times


Fig. 2. Layered schematic of the different components of the SAGA landscape. At the topmost level is the simple integrated API which provides the basic functionality for distributed computing. Our BigJob abstraction is built upon this SAGA layer using Python API wrapper

on velocities from the CFD grid is imposed on particles in the zone through dynamically constrained equation of motion for MD. As illustrated in Fig. 1, the coupling mechanism is the key component for successful hybrid CFD/MD simulations and our implementation follows the literature [6], [7].

As clearly indicated in Fig. 1, the most prominent computational challenge is how to run efficiently two separate stand alone applications while efficiently conducting information exchange. In other words, the time-to-solution is heavily dependent upon whether a runtime environment can provide, (i) low collective-waiting times (arising from batch queue wait times), and (ii) prevent an imbalance in the time to reach the information exchange step between the two codes. The imbalance arises due to difference in performance between two distinctly heterogeneous applications, CFD and MD, resulting in an unavoidable time gap between arrival times of CFD and MD for the exchange step. We propose to address this using dynamical resource allocation mechanism with a load-balancing mechanism. In that sense, our SAGA-based framework provides a single efficient runtime environment for the coupled simulation.

III. SAGA and SAGA-based Frameworks for Large-Scale and Distributed Computation

The Simple API for Grid Applications (SAGA) is an API standardization effort within the Open Grid Forum

(OGF) [10], an international standards development body concerned primarily with standards for distributed computing. SAGA provides a simple, POSIX-style API to the most common Grid functions at a sufficiently high-level of abstraction so as to be independent of the diverse and dynamic Grid environments. The SAGA specification defines interfaces for the most common Grid-programming functions grouped as a set of functional packages (Fig. 2). Some key packages are:

- File package - provides methods for accessing local and remote filesystems, browsing directories, moving, copying, and deleting files, setting access permissions, as well as zero-copy reading and writing
- Job package - provides methods for describing, submitting, monitoring, and controlling local and remote jobs. Many parts of this package were derived from the largely adopted DRMAA specification.
- Stream package - provides methods for authenticated local and remote socket connections with hooks to support authorization and encryption schemes.
- Other Packages, such as the RPC (remote procedure call) and Replica package

Fig. 3 shows the structure of BigJob and its operation flow. When a BigJob is submitted to the remote resource, the application manager monitors the status of this pilot-job through the advert service. When resources are allocated to the BigJob, the application manager allots the obtained resources to its sub-jobs and a coupled simulation starts under the control of a multi-physics agent in the remote resource. Advert service keeps on getting the status of a pilot-job from the queuing system and the status of sub-jobs from multi-physics agent and also delivers this information to the application manager by a push-pull mechanism. The application manager watches the status of sub-jobs and decides the next event when the coupled simulation is finished. When one default BigJob
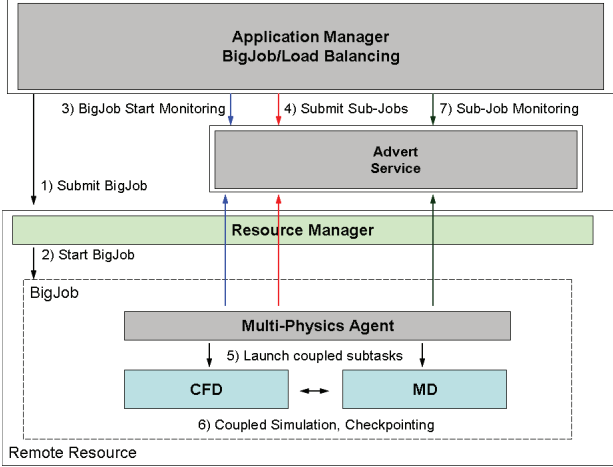
Fig. 3. Architecture of the Controller/Manager and Control Flow: Application manager is responsible for job management including BigJob and sub-job submission, their status monitoring functions. We implement a load balancing module, and migration service based on job information. Application agent system resides on each HPC resource and conducts job information gathering and also communicates with the application manager via the advert service

is launched, sub-jobs keeps running until final solution is achieved and the manager quits the Pilot-Job at that time. In case multiple BigJobs are submitted for the same simulation or if a load balancing function is included, sub-jobs experience several restarts from their checkpointing data, reflecting changed processor allocation to each application. In the former case, resource allocation to each sub-job follows a pre-defined map according to the number of BigJobs allotted to the simulation; in the latter case, resource allocation to each sub-job becomes dynamic according to its performance, as discussed in the next section.

IV. Load Balancing for Coupled Multi-Physics Simulation

The flexibility to re-distribute resources (processors) to the individual task does not imply efficient utilization. This is the responsibility of a load-balancer (LB). We will discuss the implementation and algorithm of this LB [11]; it is important to mention that the LB functions in the context of the SAGA-BigJob framework.

Each application's load is determined by its elapsed time to run the evolution loop. Here, time for initialization or inter-domain data exchange are excluded from the counting, because they are one-time events or irrelevant to application's performance. The efficient functioning of the LB is predicated on application codes being able to restart from their checkpointing data effectively. Also,

application codes should be equipped with generalized domain partitioning routine to run a simulation with any number of processors, without harming their parallel efficiency a lot. If above conditions are satisfied, it makes sense to load the LB within the pilot-job, to implement dynamic resource allocation between tasks. Conceptually, the load-balancing algorithm assigns more processors to a sub-task with greater runtime, until the two codes take the same wall-clock time between points when they communicate. Interestingly, our approach is very simple and the algorithm is indepenendent of applications upon the predications of, (1) each application code follows the ideal parallel efficiency. (2) all processors in one node are assigned to one single task.

Let the computation time (between exchanges) of the two sub-jobs be t_{CFD} and t_{MD}, and the number of processors assigned to each domain be PE_{CFD} and PE_{MD}, respectively. Subscripts I and F denotes initial and final states. Based on assumption (1), total problem size of each application remains the same after resource re-allocation,

$$
\begin{aligned}
W_{CFD} &= PE_{CFD,I} \times t_{CFD,I} = PE_{CFD,F} \times t_{CFD,F} \\
W_{MD} &= PE_{MD,I} \times t_{MD,I} = PE_{MD,F} \times t_{MD,F} \quad (1)
\end{aligned}
$$

In spite of the re-allocation, the total number of processors utilized remains the same:

$$ PE_{TOT} = PE_{CFD,I} + PE_{MD,I} = PE_{CFD,F} + PE_{MD,F} \quad (2) $$

Our objective is to reduce the computation time of a sub-job to the point until the two application components show the same computation between the exchange points, i.e., $t_{CFD,F} = t_{MD,F}$. From Equation 1 and Equation 2 an optimal number of processors distributed for the CFD subtask would be:

$$ PE_{CFD,F} = \frac{W_{CFD}}{(W_{CFD} + W_{MD})} \times PE_{TOT} \quad (3) $$

The MD simulation (sub-job) will follow a similar expression. The optimal processor distribution from above equation will return a non-integer value. Also, under the second assumption (which is the policy of many supercomputing centers), any load-balancing determined as above, will proceed in discrete values expressed as the multiples of the number of CPU cores in a node. We choose the nearest discrete number to our load balancing as the optimal number of processor on each application.

## V. Dynamic Resource Allocation for Coupled Simulations: Experiments and Analysis

In Section 2, we outlined the challenges of running a coupled multi-physics simulation using conventional queuing systems as the following: (i) Difficulty of starting

multiple applications concurrently; (ii) Inability to balance the load among domains, and (iii) Fixed number of allocated resources throughout the simulation. To address these challenges we use the BigJob abstraction with a load balancing (LB) module for dynamic resource allocation.

We outline three possible scenarios. In the first scenario, a single BigJob is utilized to run the coupled simulations, with and without LB (denoted as $S1_{LB}$ and S1 respectively) redistributing resources based upon their individual performance. In the second scenario (S2) there are two BigJobs, and although they are started together, most often one BigJob starts before the other; to increase efficiency, both coupled simulations start with whatever resources are available as part of the first (to run) BigJob. When the second BigJob becomes active, there is a dynamic redistribution of tasks, such that the larger of the two sub-jobs is assigned the bigger BigJob. Variant of the above, when the two BigJobs are on two different machines forms the third scenario (S3). In the remainder of this section we discuss the details of these three different Use Cases.

A. Description of Experiments

Figure 4 shows two different scenarios: the first (left-most) shows the time evolution of a coupled simulation executing after using a conventional job submission (which we define to be scenario S0), and the other using a BigJob. For S0, individual tasks with resource requirements of PE_{CFD} and PE_{MD} respectively, are independently submitted to the conventional queuing system and job scheduler recognizes these coupled tasks as two distinct jobs. Thus, they are start at different times on average, except when coincidentally resources for both are available. In this case, both tasks wait on the queue when no job is allocated, the first allocated job idles to perform data exchange with its counterpart; the actual simulation executes only after both jobs are running/allocated. On the other hand, for scenario S1, a BigJob of size $PE_{CFD} + PE_{MD}$ is submitted to the queue, and coupled simulation directly starts when the resource is assigned to this BigJob. Because of co-scheduling of sub-jobs, a BigJob is free from long inactive mode which is frequent in conventional job submission, while total runtime is the same if the resource distribution to sub-jobs is identical. However, eliminating inactive mode in of itself does not guarantee a reduction in the total runtime, because a larger allocation may result in a greater queue waiting time than two simulations requesting smaller number of processors each (but the total being the same). The same situation can arise for the load-balanced case with one BigJob. Figure 5 illustrates scenarios S2 and S3 – whereby 2 BigJobs are submitted as opposed to 1 BigJob. In S2 both BigJobs are on the same machine, whilst in S3 they are on different machines. Compared
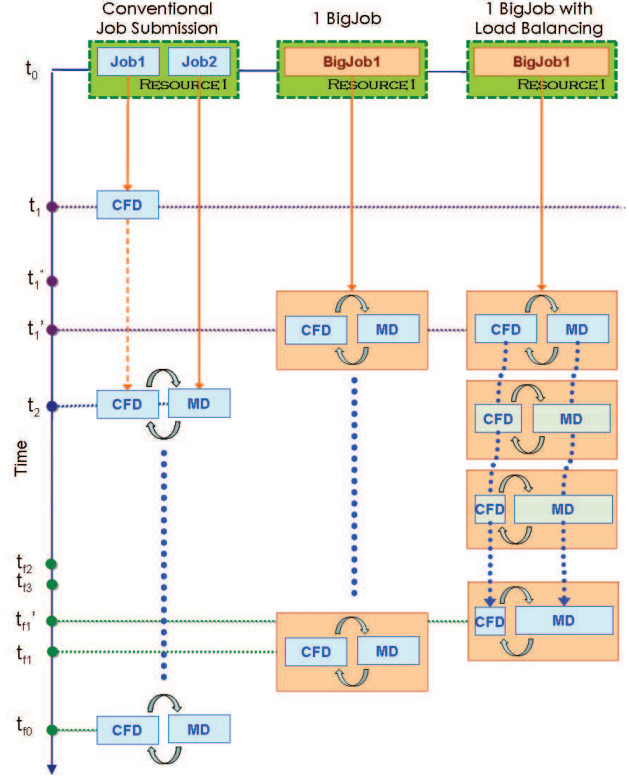

Fig. 4. Comparison of dependencies encountered for coupled simulations submitted as conventional jobs, to the scenario when using Pilot-Jobs. Here we use only 1 BigJob (S1). The conventional mode of submission experiences three phases based upon their queue state: (i) All jobs are waiting: $(t_1 - t_0)$; (ii) Inactive mode (where one job is waiting for another: $t_2 - t_1$), and (iii) Active mode (running a coupled simulation: $t_f - t_2$). The Inactive stage, disappears when a coupled simulation runs within a BigJob, as an allocated BigJob distributes its resource to both sub-jobs.

to S2, S3 is more likely to get assigned with the second BigJob faster, while the active runtime will increase a little due to the slower communication between sub-jobs in distributed resources.

We investigate a simple couette flow (Fig. 1) as the representative physical problem, to validate the performance gains and resource flexibility of above scenarios. The current flow system is composed of 62,400 mesh points (CFD) and 23,188 particles (MD). In order to reach convergence, the coupled simulation runs for a physical time of 2500τ, which is the time unit related to the characteristics of molecules. This is equivalent to 25,000 CFD iterations and 500,000 MD integration steps. During the simulation, both codes components update their boundary values by exchanging their numerical data via files, once every 10 τ. This leads to 250 synchronization steps between two simulation components over the course
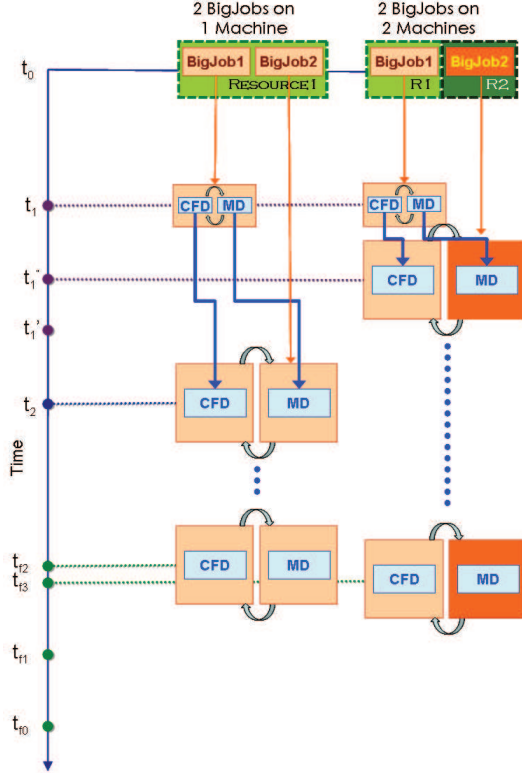
Fig. 5. Schematic comparing the distribution of simulations when 2 BigJobs are used. On the left side, both BigJobs are submitted to the same physical machine (S2); on the right side they are submitted to different (distributed) machines (S3). In both cases, coupled sub-jobs start running when the first BigJob is allocated at $t = t_1$; there is a resource reallocation when the next BigJob becomes available. When two BigJobs are allocated, each sub-job occupies a BigJob, and data exchange between jobs takes place across BigJobs.

of a single simulation run. For a rigorous test of a load balancer, larger coupled simulation task (which has 150 times more workload on CFD domain and 50 times on MD) also has been experimented.

No changes in the application codes were required in order to utilize the BigJob capabilty; however, in order to utilize load-balancing features or dynamic-resource assignement the application codes need to be equipped with the ability to carry out application-level checkpointing. The application codes in addition to having application-level checkpointing need generalized domain partitioning method to work with a range of processor counts. In the current work, the application codes experience five launch/re-launches (25 times in larger simulation) to get assigned with changed number of processors, either by the result of load balancing or more resource allocations.

The use of a load balancing function requires one more change on application codes. As load balancer refers to

the performance data from application codes, application codes need to return their actual runtime, which excludes idle waiting on inter-domain information exchange. This can be implemented by checking elapsed time on inter-domain data exchange and subtracting it from total iteration time. The use of a load balancing function requires one more change to application codes. As load balancer refers to the performance data from application codes, application codes need to return their actual runtime, which excludes idle waiting on inter-domain information exchange. This can be implemented by checking elapsed time on inter-domain data exchange and subtracting it from total iteration time.

Evaluation of the effectiveness of BigJob as a job-submission mechanism, requires carefully controlled experiments over different processor requests and different wall-time limits with varying system conditions. To understand the queue waiting time of job submissions and analyze the variation of waiting time with system's conditions under similar or controlled conditions, we define the load-factor as the ratio of the number of active nodes to the total number of nodes on the machine. We determine the effect of load-factor on queue waiting time by submitting a number of experiments to the resources and monitoring the variance of load-factor at the submission and at the allocation time. Our experiments include multiple job submissions ranging from 8 to 64 px (processors) with wall-time limit from 1 to 12 hr (hours). This waiting time issue is also discussed by simulating above coupled simulations, in a way of submitting a BigJob and two conventional jobs concurrently and counting total waiting time in both cases. Both small and large simulations are conducted using 64 px for a coupled task and wall-limit time is set to be either 6 hr or 24 hr, depending on their computation times.

Simulations used to validate and determine the performance measures were conducted on supercomputing resources on TeraGrid machines (62,976 cores Ranger), shared TeraGrid-LONI (Louisiana Optical Network Initiative) [12] machines (5,440 cores QueenBee) and some smaller LONI machines such as Eric, Oliver, Louie and Poseidon(512 cores each). We monitored the load on these systems over a long period of time (several weeks) and found Queenbee to be significantly more loaded than other resources.

B. Using Pilot-Jobs to submit Coupled Simulations: Queue Wait Time Analysis

We designed experiments to determine if running larger and/or longer simulations effects the actual waiting time on the queue. We performed our experiments on machines spanning two orders of magnitude in size (and peak

TABLE I. Effect of various configurations on waiting time. The tables show the queue waiting times on Ranger and QueenBee with a changing number of processors and different requested resource wall-time limits. Analyzing the actual waiting time as a function of the number of processors at different wall-time limits, it can be said that better more often than not, the waiting time decrease as the requested number of processors increases. The relationship between the waiting time and wall-time limit is harder to quantify. However, obtained numbers provide a good case study for showing the variance of actual queue waiting times.

Number of processors	Requested wall-time at 92±6% load (Ranger)				
	2hr	3hr	4hr	6hr	12hr
	Waiting time on the queue [sec]				
16	9989	15984	39151	65	66
32	15371	4106	11376	54	55
48	13264	4392	37780	43	44
64	9944	1975	39855	31	32

Number of processors	Requested wall-time at 95±4% load (Queenbee)				
	2hr	3hr	4hr	6hr	12hr
	Waiting time on the queue [sec]				
16	14339	3578	39113	6	940
32	14312	3550	39238	5	6344
48	21555	3517	39207	4	6353
64	21541	3489	39179	3	6329

performance)– from approximately 500 px to 65000 px, and for a range of load-factors. We submitted jobs of different sizes, requiring different wall-time limits. Each time we submitted a job, we gathered the load-factor and the actual waiting time on the queue. Many factors effect the waiting times, arguably the most important of them are the load-factor at the instant of submission, requested wall-time limit and also the number of processors requested. Two other factors that effect this are the backfilling that occurs when some other unrelated job finishes and the changes in the priority of the test job when a particular higher priority job joins the queue; however, unlike the first three factors, the last two are somewhat random and it is difficult to systematically account for them. Also, the internal queueing policy of supercomputing centers may effect the waiting time on the queue based on their queueing priority including credential, fairshare, resource and service priority. As can be seen from Table I, the waiting time tends to decrease as the number of processors requested in a job increases.

Results for machines with more than 5000 px, Ranger and Queenbee are presented in Table I, and as can be seen, jobs with larger processor counts have typically lower wait times. The observation holds true for a range of values of requested wall-times over a range of "high" load-factors.

It is however, difficult to discern a relationship between waiting time with the requested wall-time limit of jobs;

TABLE II. Waiting and inactive time for conventional job submissions, and a single BigJob submission. All measured times are in seconds and expressed as 'mean±SD'. In both cases, conventional job is submitted to use 2×32 px and a BigJob requests 64 px on small and less crowded LONI clusters. Conventional job submission mode showed faster time-to-start (i.e., the sum of waiting time and inactive mode) on small problem size with 6 hr of wall-time limit, while a BigJob gets allocated faster with longer wall-time limit. Conventional job submission showed 3 failures during the test due to the timeover of wall-time limit in the first-started job.

	Small simulation with 6 hr wall-time limit		
	Waiting time	Inactive mode	Failed runs
Conventional	12318±15649	7407±11375	2
1 BigJob	29452±31946	0	0

	Large simulation with 24 hr wall-time limit		
	Waiting time	Inactive mode	Failed runs
Conventional	83102±77134	47488±55647	1
1 BigJob	76645±55474	0	0

from experience there is greater variation in backfilling probability with varying wall-time requests. However, as we are able to establish that a single large job on average has to wait less at the queue than a smaller job does, most definitely the maximum wait time of two small jobs will be even greater. In other words the sum total of the waiting time (of the first-to-run job) and the inactive time (defined as the difference between the waiting time of the two jobs) will be larger than the wait time of a single large job.

Controlling runtime in these two scenarios, i.e., we take a BigJob of size 2X and 2 conventional jobs of size X each, we compare the waiting time of a 64 px BigJob (with wall-clock limits of 2, 3, and 4hrs) which is smaller than the wait for a 32 px conventional job for the same values of wall-clock limits. As the individual simulations are assigned the same number of processors, the runtime performance will be similar in the two scenarios, and thus the total time-to-solution will determined by the wait-times on queues – which we show statistically to be lower for the larger BigJob submission mode.

Results for smaller systems ($\approx$ 500 px) are presented in a different fashion in Table II. In addition to the fact that a 64 px BigJob is now around 16% of the machine resources, the load-factors of the smaller machines fluctuated much more than those of the larger machines. Consequently the data obtained for smaller resources is far more noisier and than the "clean" data for the larger machines – Ranger and QueenBee. As can be seen from Table II although the waiting time for the first-to-start job was smaller in the conventional job submission mode than the BigJob (S1), the second job (convention job) had a large subsequent wait time; thus for conventional job

TABLE III. Results of runtime for S1, $S1_{LB}$ and conventional submission. All measured times are in seconds and expressed as 'mean±SD'. 6 distinct experiments were accomplished for each simulation, all with 64 px. In both cases, S1 shows about 1% overhead due to the communication with advert server. On the other hand, $S1_{LB}$ tests show about 13% runtime save compared to conventional submission.

	Conventional	S1	$S1_{LB}$
Small sim.	757±1.89	764±1.41	661±4.41
Large sim.	39595±119.2	39906±206.3	34350±1302.7

submission mode there is a non-negligible inactive mode (defined as the time difference between queue wait times between the two simulations). There is no inactive mode for BigJob submission as by defintion both simulations begin concurrently. Interestingly, the situation is somewhat worse for the conventional job submission; although the average wait time is lower than the BigJob, there exist 2 (out of 6) cases (for 6hr wall-clock limit), when the wait time of the second job is greater than the wall-clock limit for the first-to-start job. In other words, the second job fails to start in the duration that the first-to-start job is in active/run mode, but can't do anything useful as the second job is still waiting on the queue. This is typically alleviated with co-allocation of resources; however the number of production grid infrastructure that provide co-allocation (and co-scheduling) as a production service is very limited. This leads us to the heart of the advantage of the BigJob submission mode: circumventing the requirements of co-scheduling by providing an application level solution that preserves performance and guarantees non-failure due to large-fluctuations (see data for 24hr wall-time limit) in queue waiting times.

C. Scenario S1: Pilot-Job with Load Balancing

Runtimes of the coupled simulation with a single BigJob is given on Table III. For both small and large simulations, a default BigJob task takes about 1 percent longer than the conventional test. This is reasonable because a default BigJob has the same processor distribution between sub-jobs as the conventional job, while BigJob has the minor overhead of sub-jobs' status monitoring and communication with advert server. In cases of load-balanced BigJob simulations, there is a significant reduction in the runtime compared to successful conventional jobs – 13% and greater. For larger problem set, a load-balanced BigJob simulation relatively shows higher standard deviation (SD) due to the unexpected instability of a computing resource during one experiment, to be discussed in detail below.

The validity of a load balancing function can be discussed by the change of processor distribution between
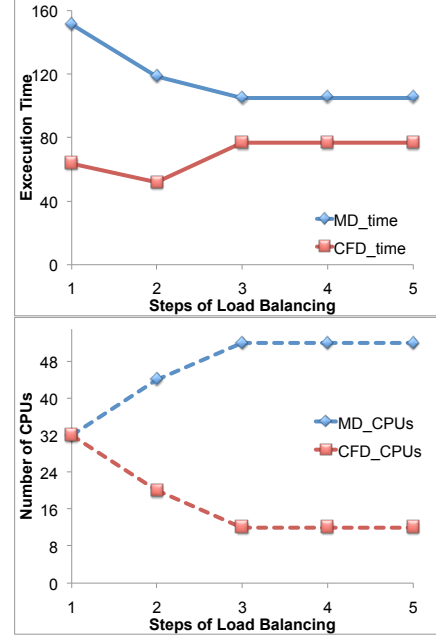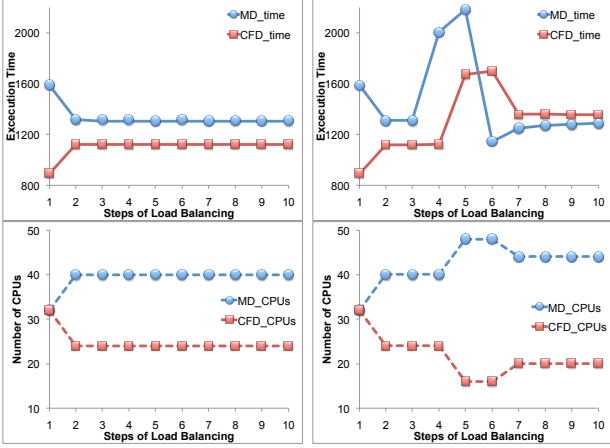

Fig. 6. Change of processor distribution between CFD and MD jobs and resultant computation time in the small simulation. A load balancer starts from the same number of processors assigned to both sub-jobs and detects 20 to 44 px between each sub-job as the optimal solution. The poor scalability of CFD job makes the load balancer to search for the optimal condition once again and the processor assignment finally reaches to a steady solution of 12 to 52 between two sub-jobs. Computation time for every simulation loop reduces from 153 sec to 107 sec after the balancing.

subtasks throughout the simulation. For the result of a small simulation in Fig. 6, both CFD and MD subtasks are assigned with 32 px initially. After two simulation loops, a load balancer converges to the processor distribution of 12 to 52 px between CFD and MD respectively; this processor distribution remains the same until the simulation completes. Runtime per loop is reduced from 153 sec for the first loop to 107 sec after the convergence. Total computation time is 596.19 sec, which is different from 663 sec counted from BigJob application manager. This time difference implies that the BigJob application manager spends about 13 sec per stage in executing its internal commands including the run of a load balancing function and sub-job re-launch.

The result of computation time evolution for a large simulation is seen in Fig. 7. For most experiments, which is given in the left side of Fig. 7, a load balancer directly goes to a converged solution of processor distribution, which is 24 to 40 between CFD and MD jobs. On the other, in one experiment, computing nodes assigned to MD simulation seem to have temporarily experienced the internal overhead as shown from the right side of Fig. 7. This overhead

Fig. 7. (Left Column) Change of processor distribution between CFD and MD jobs and resultant computation time in the large simulation. A load balancer directly finds the processor distribution of 24 to 40 between CFD and MD jobs and remains the steady state until it completes after 25 simulation loops. Initial computation time of 1605 sec reduces to 1320 sec after the convergence. (Right Column) Plots showing non-monotonic resource assignment by the LB, and thus demonstrating how the load balancer can be self-correcting and adapt to changing performance; after increasing the number of processors assigned to the MD, the load-balancer unassigns the additional processors.

temporarily increased MD computation time a lot and a load balancer shows the fluctuating pattern of processor distribution in response to this temporary instability. A load balancer goes to a different steady solution after the system settled down, which is the processor distribution of 20 to 44 between two sub-jobs. Compared to the steady solution in stable cases, computation time for one simulation loop increases in this processor distribution increases from 1320 sec to 1380 sec. Plots on the right side of Fig. 7 show a non-monotonically changing resource assignment by the LB, and thus demonstrating how the load balancer can be self-correcting and adapt to changing performance; after increasing the number of processors assigned to the MD, the load-balancer unassigns the additional processors.

D. Scenario S2 and S3: Logically and Physically Distributed Pilot-Jobs

In Table IV, results from the four test runs representing scenarios S2 and S3 using two BigJobs are presented. The general setup for scenarios S2 and S3 is that when two BigJobs are submitted, one BigJob becomes active first and the other BigJob becomes available later – either on the same resource (S2) or on another resource (S3). The MD and CFD request half of each BigJob. When the second BigJob becomes active, each application is immediately configured to run in each BigJob so as to consume all BigJob CPUs. Therefore, more CPUs allow each application to speed up. Conceptually the LB scheme adopted for S1 can be trivially applied here, but for simplicity and as proof-of-concept, we confine our test runs to the configuration in Fig. 5, i.e., without a load balancing scheme to determine an optimal distribution of resources.

TABLE IV. Performance measured for Scenarios S2 and S3 (2 BigJobs on 2 different machines). Here, we present the time to solution in terms of two components, T_{comm} and $T_{compute}$. The details on how to conduct these experiments are described in the text. All measured time are in seconds. BigJob size refers to the size of two BigJobs as determined by the number of requested cpus. Resource describes the system used (L stands for Louie; P for Poseidon. L & P are LONI resources)

Test	1	2	3	4
Scenario	S2	S2	S3	S3
BigJob size	(8,16)	(8,16)	(8, 16)	(16,32)
Resource	P	L	L + P	L + P
1 BigJob				
$T_{compute}$	1037.2	1045.2	1049.0	534.2
T_{comm}	0.006	0.010	0.912	0.957
2 BigJob				
$T_{compute}$	277.2	277.8	276.8	150.4
T_{comm}	0.041	0.009	0.990	0.60

As shown in the table, the results with these four test cases clearly demonstrate performance gains with additionally available cpus when two BigJobs. The performance gain is examined with respect to two components T_{comm} and $T_{compute}$ of the total time-to-solution. $T_{compute}$ represents the maximum of $(T_{MD,compute}, T_{CFD,compute})$ – which is the longer compute time of two applications, andby the start time and the end time between the data exchange. As more cpus become available with the incoming BigJob, more gain in the performance is achieved as shown in the case of test 4. On the other hand, the time for communication, T_{comm} is further decomposed into $T_{read-write}$ and $T_{file-transfer}$. Note that the latter is only required with S3. There are other components that contribute to the overall time-to-solution, such as the waiting time in queue etc., but are not considered here to focus on the performance gain arising from simple dynamic execution (resource allocation) as illustrated from S2 and S3.

According to our results, the communication time is insignificant even for S3 – thanks in part to the small size of the data required to be exchanged. Of course, the file transfer depends heavily on the network condition, but it is not expected to become a major issue considering the observation that T_{comm} is a tiny fraction of $T_{compute}$. Furthermore, we expect that the ratio of the two components will remain similar, or if anything becomes larger (i.e.,

T_{comm} becomes less significant) as the size of physical system simulated increases, i.e., the number of particles in MD or the number of mesh points increases. Indeed, the development of an efficient runtime environment for hybrid CFD/MD simulation lies in finding a way to decrease $T_{compute}$. Arguably, the results in the table IV suggest that a BigJob-based runtime environment is able to provide a reasonable solution to this end.

VI. Conclusions

In this work, we report the first production application-level framework that uses generalizations of the Pilot-Job to enable an efficient runtime environment targeting coupled multi-physics application comprising MD and CFD. It is not trivial to integrate a targeted scientific application with a resource management system that is aware of the challenges arising from the distribution – logical and/or physical, well as the local scheduler implemented with the local resource management policy. Overcoming the co-scheduling requirements and implementing dynamic resource allocation mechanism were two main goals motivating a novel development and our test runs demonstrated its potential for large scale scientific simulations benefiting scientific problems that are only tackled by a coupled hybrid MD-CFD calculation. Our development is built upon the BigJob framework enabled by the SAGA which provides a simple and consistent interface for managing HPC resources and natively supports an agile and flexible execution model.

We validated and tested development for performance on three cases and demonstrated its capability. Our approach is minimally intrusive towards the application code. Using MPI as a coupling layer would also require code modification, adding infrastructure to support simulation-to-simulation communication. To maintain a high level of adaptivity, abstraction, interoperate between various application codes, and to eliminate application code invasion, we opted not to use MPI and focus on non-invasive abstract coupling layers. Some of these problems arise from the nature of the simulations: large scale simulations that would not be able to run concurrently on the same resource, while others issues are quite technical such as dynamic shrinking/expanding the number of MPI processes of each application (dynamic load-balancing).

In summary, we have established that the use of a BigJob as a container for coupled-simulations is an effective approach. Not only is runtime performance preserved, but in the absence of production grade co-scheduling/co-allocation service, there is a significant reduction in the waiting time and a complete elimination of failed runs due to excessive long queue waiting times. Also, the BigJob framework supports the use of a load balancing function, which enables coupled codes to use the allocated resources more efficiently. We have established that the performance advantage of using BigJobs is invariant with the size of the machine, i.e., small LONI machines such as Eric, to the largest machines available such as Ranger. This claim is valid not only as machines get larger, but also for progressively larger physical models that we are investigating. We will report results on these in the near future.

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