Using Cross-Layer Adaptations for Dynamic Data Management in Large Scale Coupled Scientific Workflows

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ABSTRACT

As system scales and application complexity grow, managing and processing simulation data has become a significant challenge. While recent approaches based on data staging and in-situ/in-transit data processing are promising, dynamic data volumes and distributions,such as those occurring in AMR-based simulations, make the efficient use of these techniques challenging. In this paper we propose cross-layer adaptations that address these challenges and respond at runtime to dynamic data management requirements. Specifically we explore (1) adaptations of the spatial resolution at which the data is processed, (2) dynamic placement and scheduling of data processing kernels, and (3) dynamic allocation of in-transit resources. We also exploit coordinated approaches that dynamically combine these adaptations at the different layers. We evaluate the performance of our adaptive cross-layer management approach on the Intrepid IBM-BlueGene/P and Titan Cray-XK7 systems using Chombo-based AMR applications, and demonstrate its effectiveness in improving overall time-to-solution and increasing resource efficiency.

Categories and Subject Descriptors

H.4 [**Information Systems Applications**]: Miscellaneous; C.2.4 [**Computer - Communication Networks**]: Distributed Systems; D.2.8 [**Software Engineering**]: Metrics—*performance measures*

Keywords

Cross-layer adaptation, in-situ/in-transit, coupled simulation workflows, staging, data management

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1. INTRODUCTION

Advanced coupled simulation workflows running at extreme scales are providing new capabilities and new opportunities for insights in a wide range of application areas.

These workflows compose multiple physical models and codes along with data processing and analysis services, and are presenting new challenges due to their scales, coupling and coordination behaviors and overall complexities, which must be addressed before their potential can be fully realized. For example, many of these simulations are based on dynamically adaptive formulations such as Adaptive Mesh Refinement (AMR), which exhibit dynamic runtime behaviors and result in large and dynamically changing volumes of data. Efficiently managing, transporting and analyzing this data has become a significant and immediate challenge.

Recent approaches based on data staging [5, 6, 16] and in-situ/in-transit data processing [25, 3] that are attempting to address these challenges are promising – these approaches offload data processing to separate resources on the same systems (in-transit) and/or perform the processing directly on the resources that are running the simulation (in-situ). For example, our previous work [3] demonstrated how a simulation plus analytic workflow can efficiently execute on a high-end computing system using a hybrid in-situ/in-transit approach. Specifically, we proposed to decompose the analytic components of the workflow into pieces that can run scalably in-situ, and pieces that run in-transit – e.g., the raw data is down-sampled in-situ using a predefined sampling rate and is then transported to the in-transit for further analysis. The effectiveness of this approach clearly depends on the mapping of workflow components, the size and distribution of the data and the resources available in-situ and in-transit, and achieving efficiency and scalability requires carefully configuring the staging resources mapping based on application behaviors. While these can be preconfigured for relatively simple and static workflows, such an approach becomes ineffective when application behaviors become dynamic, as is the case for AMR-based simulations

– in AMR-based simulations, dynamic refinements can lead to imbalanced data distributions and heterogeneous resource (memory, CPU, network bandwidth) requirements.

In this paper we explore cross-layer adaptive runtime approaches to address these challenges. Specifically, we explore runtime adaptations at three different layers - application layer, middleware layer, and resource layer. We evaluate their ability to respond to the dynamic data processing requirements and resource constraints in a coupled AMR-based simulation workflows. At the application layer, we can dynamically adapt the spatial and temporal resolution of the data being written and processed; at the middleware layer, we can adapt the in-situ/in-transit placement and the scheduling of data processing operations; and at the resources layer we can adapt the allocation of in-transit resources. We then explore a coordinated approach that combines these adaptations in a cross-layer manner to optimize the end-to-end performance of the workflow.

We have implemented the adaptive cross-layer management approach on the Intrepid IBM BlueGene/P system at Argonne National Laboratory and the Titan Cray-XK7 system at Oak Ridge National Laboratory. We use these systems with a Chombo [1]-based AMR simulation plus data visualization workflow to experimentally evaluate the behavior of the individual adaption at each layer, as well as the effectiveness of the dynamic and coordinated cross-layer approach in improving overall time-to-solution, increasing resource efficiency, and mitigating I/O costs.

The rest of this paper is organized as follows. Section 2 presents the data management challenges in advanced coupled simulation workflows and highlights the challenges of the Chombo [1]-based AMR simulation plus data visualization workflow. Section 3 describes the conceptual architecture and operation of the adaptive cross-layer management approach and its components. Section 4 develops specific adaptation policies. Section 5 presents the results of our experiments using the Chombo-based application workflow on Intrepid and Titan. Section 6 discusses related work. Section 7 concludes the paper and outlines future work.

2. PROBLEM DESCRIPTION

As noted above, dynamically adaptive simulation formulations such as those based on Adaptive Mesh Refinement (AMR), exhibit dynamic runtime behaviors and result in large and dynamically changing volumes of data, imbalanced data distributions and heterogeneous resource (memory, CPU, network bandwidth) requirements. Figure 1 shows peak memory consumption for an AMR-base simulation using Chombo library. Although memory consumption increases for each time step, the pace in which the memory consumption increases is erratic. Moreover, the memory usage is not distributed evenly among these processes. These characteristics increase the complexity of managing staging resources and scheduling in-situ/in-transit data processing while satisfying constraints on the amount of data movement, the overhead on the simulation, or/and the level of analytics.

For example, AMR-based simulations involve dynamic local refinements which can significantly increase the resources consumed by the simulation on a subset of nodes. This in turn reduces the available resources for in-situ analytics. At the same time, it also increases the spacial-temporal resolutions of data and the computational/data requirements

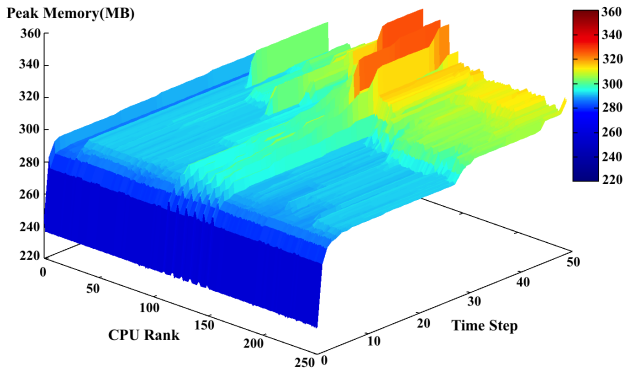


Figure 1: Distribution of peak memory consumption for an AMR-based Polytropic Gas simulation using the Chombo library.

for the analytics, as well as the cost of data movement if the analytics have to be executed in-transit. The increasing computational/data requirements of the analytics can also impact in-transit resource requirements. Note that as the simulations evolves, refined regions maybe further refined or coarsened.

To further illustrate the dynamic data management and processing requirements of AMR-based simulations, consider the *3-D AMR Polytropic Gas* application that is part of the Chombo package [1] developed by Lawrence the Berkeley National Laboratory. This application implements the Godunov unsplit algorithm for integrating systems of conservation laws (e.g., the Euler equations of gas dynamics). Figure 1 plots parts of a profile of the distribution of the application's peak memory usage on 4K CPU cores over 50 time steps. As we can see from this plot, memory usage varies significantly, both across cores and over time. More importantly, the peak memory usage can be as high as several Gigabytes per node if multiple memory hungry process are placed in the same multi-cores node.

Clearly, making staging and in-situ/in-transit processing approaches effective for these dynamic applications given performance, overhead and resource constraints requires runtime trade-offs and adaptations at different levels. Adaptations may be explored at different levels. At the application level, the application may be able to adapt the spatial and/or temporal resolution of the analytics or limit the analytics to "interesting" regions, to meet the constraints on the type of analytics, the available resources and/or acceptable overheads. Similarly, at the runtime level, the placement and scheduling of in-situ/in-transit tasks can be adapted and at the resource level, the number of in-transit resources can be adapted. In this paper we explore how we can realize these dynamic adaptations at runtime for AMR-based simulation workflows on large-scale systems. We also explore policies and mechanisms for combining these adaptations in a coordinated and cross-layer manner to better address application requirements and constraints.

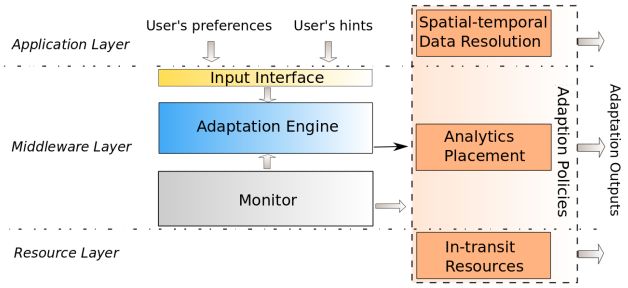


Figure 2: A conceptual architecture for realizing runtime adaptations for in-situ/in-transit implementations of coupled simulation workflows.

3. REALIZING CROSS-LAYER ADAPTATIONS FOR LARGE-SCALE SIMULATION WORKFLOWS

This section describes our approach for efficiently and scalably realizing runtime adaptations for in-situ/in-transit implementations of coupled simulation workflows. The conceptual architecture follows an autonomic approach and consists of three key components, a monitor, the adaptation engine and adaptation policies, as illustrated in Figure 2 and described below. In our approach, users can provide two types of inputs. *User preferences* define the objectives that users expect to achieve, such as minimizing time-to-solution, minimizing data movement, using highest available data resolution, etc. *User hints* provide additional information to adaptation the engine based on the user's knowledge of the application workflow and on past experience, for example, toleration to data downsampling, nature of regions of interest, possible adaptation phases and/or patterns, etc.

The *Monitor* captures runtime status information at the different layers (application, middleware, and resource) and uses it to characterize the current operational state of the system and application, and trigger adaptations if appropriate. Status information includes resource utilization and resource availability (memory, bandwidth, CPU cores) as well as application execution time, analysis time and the size of the generated data. The *Adaptation Engine* is responsible for selecting and executing appropriate adaptations based on user preference and hints, operational state provided by the monitor, and the adaptation policies.

Three adaptation mechanisms are currently defined. In the first mechanism, the application layer changes the spatial and/or temporal resolution of data generated in-situ before its is moved to the in-transit resources for processing. This mechanism can adjust the frequency of in-situ data reduction as well as the type of reduction performed by appropriately selecting the parameters of the data reduction module (e.g., down-sample factor, compression rate, etc.). The second adaptive mechanism adapts the placement of the data processing operation at middleware layer. Placements can be in-situ, in-transit or hybrid (in-situ + in-transit). The third adaptation mechanism targets the resource layer, determines the number of in-transit resources and dynamically allocates resource for in-transit processing if required.

The *Adaptation Policies* specify which adaptation mechanism(s) should be executed based on user inputs and the operational state. In the following Section, we develop adaptation policies at each of the layers as well as a policy for combined cross-layer adaptation.

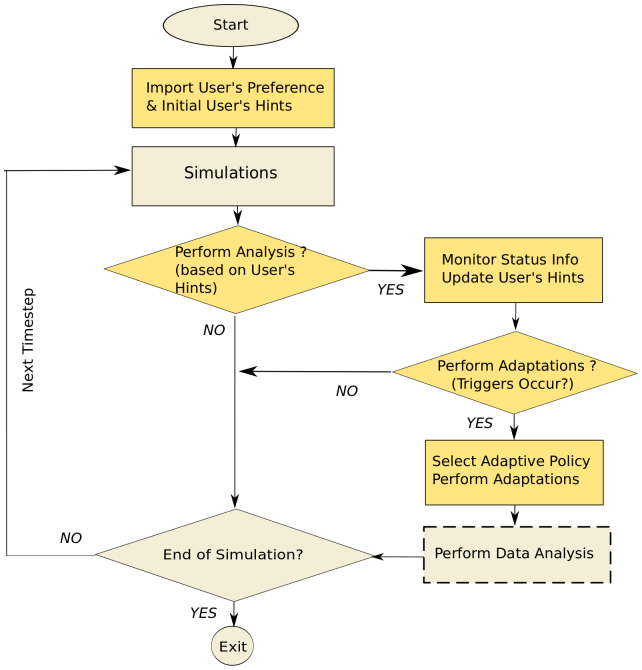


Figure 3: An overview of the adaption process.

The adaption process is illustrated in Figure 3. The operational status of the simulation workflow is periodically (e.g., after every specified number of simulation time steps) sampled by the*Monitor* and forwarded to the *Adaptation Engine*, which determines if an adaptation is required and triggers the appropriate adaptation(s).

4. DEFINING ADAPTATION POLICIES

In this section, we develop adaptation policies for an AMR-based simulation workflow. Note that rather than find optimal adaptations, our goal is to develop policies that can be efficiently and scalably implemented at runtime on very large scale system. Specifically, we develop policies for each of the 3 layers as well as a cross-layer policy of coordinated adaptations, which are described in the following subsections. Table 1 summarizes the notation used in this discussion.

4.1 Policy for Adaptation at the Application Layer

The application layer adaptive mechanism controls the resolution of the data that is forwarded to the analysis methods, and enables a trade-off between the time and resources spent on analysis and the resolution at which the analysis is performed. For example, it may be beneficial to have some analysis done even if it is performed at a lower resolution. The goal of this adaptation is to determine the data resolution that can be effectively processed in-situ or transferred to in-transit resources given the user preferences and current operational state. Specifically, it determines the factor(X) by which to downsample the simulation data. This is selected from a set of acceptable downsampling factors provided by the user as a hint, or generated automatically based on information content of interest. The selec-

S_{data}	size of simulation output	(1)(8)(10)
X	down-sampling factor	(1)(3)
$f_{data\_reduce}(S_{data}, X)$	data reduction operation	(2)
$Mem_{data\_reduce}(S_{data}, X)$	memory needed to perform data reduction	(2)
$Mem_{available}$	total available memory	(2)
T_{sum_insitu}	total wallclock time on in-situ resources	(4)(6)
$T_{sum\_intransit}$	total wallclock time on in-transit resources	(5)(6)
N	number of simulation processors	(4)
M	number of in-transit processors	(5)
$ITER$	total number of iterations	(4)
D_i	final decision on performing analysis code: 1 for in-situ, 0 for in-transit	(4)(5)(7)(8)
$T_{i\_sim}(N)$	execution time of the ith iteration of the simulation	(4)(9)
$T_{i\_insitu}(N, S_{i\_data})$	execution time for the ith in-situ analysis on N processors	(4)(7)
$T_{i\_intransit}(M, S_{i\_data})$	execution time for the ith in-transit analysis on M processors	(5)(9)
$T_{i\_intransit\_wait}$	idle time on the in-transit side	(5)
$T_{i\_insitu\_wait}$	idle time on the in-situ side	(4)
$T_{j\_intransit\_remaining}(M, S_{j\_data})$	remaining execution time for the jth iteration in-transit processing	(7)
$Mem_{insitu}(S_{i\_data}, N)$	memory cost for in-situ processing	(8)
$Mem_{intransit}(S_{i\_data}, M)$	memory cost for in-transit processing	(8)(10)
$T_{i\_sd}(S_{data})$	the latency for sending data	(9)
$T_{i\_recv}(S_{data})$	the latency for receiving data	(9)

Table 1: Notation used in defining adaptation policies and formulation index.

tion is made based on the available memory and the memory need to implement downsampling factor X, and the smallest value of X that can be used given the memory constrains. The downsampling factor for the i^{th} simulation iteration is determined by the following policy:

Maximize

$$S_{data} - f_{data\_reduce}(S_{data}, X) \tag{1}$$

Subject to

$$Mem_{data\_reduce}(S_{data}, X) \leqslant Mem_{available} \tag{2}$$

(memory requirement)

$$when X \epsilon \{X_1, X_2, \cdots, X_n\} \tag{3}$$

(set of acceptable down-sample factors)

4.2 Policy for Adaptation at the Middleware Layer

Adaptations for middleware layer target target the placement of the analytics either in-situ or in-transit to minimize the overall time-to-solution under the current resource constraint. The policy is triggered in three cases: (1) If there are sufficient memory resources to perform the analysis either in-transit or in-situ, the adaptation will place the analysis at the location where memory resources are available. (2) If there are sufficient memory resources at both locations and in-transit CPU resources are available, the analysis will be placed in-transit since the analysis can run in parallel with simulation. (3) If the in-transit cores are busy processing simulation data generated at previous time steps, the adaptation will simply estimate the remaining time for such in-transit data processing, as well as the possible execution time if performing in-situ processing. If the in-situ data processing is estimated to be faster, the analysis will be determined to perform in-situ directly. Otherwise, the data will be asynchronously transferred to staging nodes immediately, and get processed as soon as in-transit cores become

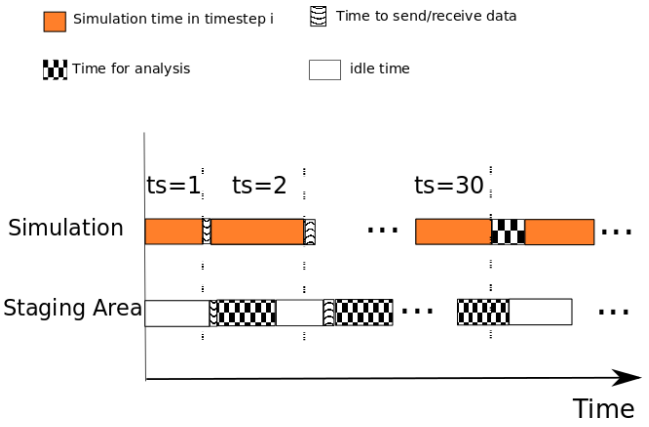


Figure 4: Demonstration of analysis placement adaptation policy. For adaptation at ts=1 and 2, in-transit processors are idle, so analysis is placed in-transit. For adaptations at ts=30, in-transit processors are busy, the analysis time of in-situ and in-transit are estimated, and the analysis is placed in-situ for shorter estimated processing time. Since data transfer is asynchronous, the time send/receive data is much smaller than the time to process data.

available. These last two cases are demonstrated in Figure 4 and can be expressed in the following formulations:

Since

$$T_{sum\_insitu} \simeq \sum_{i=1}^{ITER} \{T_{i\_sim}(N) + D_i \cdot (T_{i\_insitu}(N, S_{i\_data})) + \bar{D}_i \cdot (T_{i\_insitu\_wait})\} \tag{4}$$

$$T_{sum\_intransit} \simeq \sum_{i=1}^{ITER} \{\bar{D}_i \cdot T_{i\_intransit}(M, S_{i\_data}) + T_{i\_intransit\_wait}\} \tag{5}$$

Minimize

$$max\{T_{sum\_insitu}, T_{sum\_intransit}\} \tag{6}$$

(minimized time-to-solution)

Subject to

$\bar{D}_i \cdot (T_{j\_intransit\_remaining}(M, S_{j\_data}) < T_{i\_insitu}(N, S_{i\_data})) = 1, j < i;$ (7)

(execution time estimation)

$D_i \cdot (Mem_{intransit}(S_{i\_data}, M) < S_{data}) + \bar{D}_i \cdot (Mem_{available} \leqslant Mem_{insitu}(S_{i\_data}, N)) = 1$ (8)

(resource constraints).

4.3 Policy for Adaptation at the Resource Layer

Performing analysis in-transit minimally impacts the scientific simulation and achieves better time-to-solution. However, this approach sacrifices the computational resource to achieve the performance enhancement on overall time-to-solution because in-transit resource is often over-allocated in case of memory/CPU unavailability.

The resource layer adaptation is targeting this trade-off between maximized time-to-solution over minimized staging resources. While performing in-transit processing, the ideal time-to-solution can be achieved if in-transit analysis on simulation data generated at the ith time step finishes before the raw data of the $(i+1)$th simulation is ready to send. In other words, the less idle time the in-transit cores have, the more efficient the in-transit resources are utilized. On the other hand, enough in-transit resource are needed to cache the simulation data generated at current time step. Therefore, the adaptation initially determines the minimal number of in-transit cores accordingly based on the size of produced simulation data and required in-transit memory resource. And then, if the in-transit processing is estimated to cost more time than the simulation, more in-transit cores will be assigned adaptively to satisfy the ideal time-to-solution. This resource constraints and heuristic adaptive policy can be formulated using the following expressions.

Minimize M

Subject to

$T_{i+1\_sim}(N) + T_{i+1\_sd}(S_{i+1\_data}) = T_{i\_intransit}(M, S_{data}) + T_{i\_recv}(S_{i\_data})$ (9)

(Expected same execution time on both simulation side and in-transit side)

and

$Mem_{intransit} > S_{data}$ (10)

(in-transit memory constraint)

4.4 Policy for Combined Cross-Layer Adaptation

Given the adaptive mechanisms at all three layers, it is important to coordinate them appropriately to better achieve the cross-layer adaptation according to user-defined objectives. Better performance would be achieved if the combination of adaptations could contribute to the user defined objective, which could be minimizing time-to-solution or minimizing data movement. To utilize the potential of such combined cross-layer adaptation and evaluate its effectiveness, we propose and design a heuristic *root-leaf* policy for the selection of adaptation mechanisms at three layers mentioned in the previous sections.

There are three steps of performing this combined adaptation policy: looking up *root mechanisms*, looking up *leaf mechanisms*, and executing mechanisms. Let us take minimizing time-to-solution as an example objective to illustrate these steps of our policy. Firstly, the policy selects the mechanisms with the same objective as that of the cross-layer adaptation, and marks them as *root mechanisms*. Based on the descriptions of adaptation mechanisms at three layers, we can tell that the middleware adaptation should be included automatically since it has the same objective as that of combined cross-layer adaptation - minimal time-to-solution. Secondly, it goes through the formulation of *root mechanisms* and looks for their data dependencies with other layers' mechanisms. In this example, the data size S_{i_data} and the number of in-transit cores M are two significant input factors in *root mechanism* – middleware adaptation mechanism, and are also impacted by the application layer adaptation for data reduction and resource layer adaptation. Therefore, the mechanisms on these two layers are marked as *leaf mechanisms*. Finally, after both *root mechanisms* and *leaf mechanisms* are marked, the policy executes these adaptations from *leaf mechanisms* to *root mechanisms*. If there are data dependencies among *leaf mechanisms*, the execution will start from *leaf mechanisms* that don't reply on others' outputs, and then their dependents. Here, the application layer adaptation will be executed first since its output S_{i_data} will impact the other *leaf mechanism* – resource layer adaptation. And then, middleware adaptation will be performed at last as the *root mechanism*.

Similarly, if the user-defined objective is to maximize in-transit resource utilization, the policy will mark resource layer adaptation as *root mechanism* and the application layer adaptation as *leaf mechanism*. But the middleware adaptation will not be included since it has no data dependency with the *root mechanism*.

5. EXPERIMENTAL EVALUATION

In this section we present experimental evaluation of the adaptive runtime management approach presented in this paper. We first evaluate adaptations at each of the three levels individually, and then evaluate the combined cross-layer adaptations.

5.1 Experiment Setup

AMR-based Simulation Workflow:.

The evaluation presented in this section uses a simulation workflow that is composed of Chombo [1]-based AMR simulation and a visualization service, which are described below.

Chombo-based AMR Simulations: We use two different AMR-based simulations that are distributed as part of the Chombo AMR package [1]. Both the simulations implement the AMR Godunov unsplit algorithm but show very different performance characteristics. The *AMR Advection-Diffusion* simulation implements an adaptive conservative transport (advection-diffusion) solver, while the *AMR Polytropic Gas* implements the AMR Godunov unsplit algorithm for integrating systems of conservation laws (e.g., the Euler equations of gas dynamics). While both simulations exhibit runtime adaptations, the latter is more memory and compute intensive especially in 3-D.

Visualization Service: The visualization service implements the marching cubes algorithm [13, 21], the *de facto* standard isosurface extraction algorithm in scientific visu-

alization, to construct triangular meshes from AMR data according to user specified isovalues. The algorithm scans each cell and conducts triangulation depending only on the values of the current cell, and thus the isosurface construction is performed locally. The ghost regions are managed by Chombo, and there is nearly no communication needed for the marching cubes algorithm. We can extract isosurfaces from full-resolution data in-situ, which can generate a high-quality triangular mesh to capture the fine structural information.

Implementation of the Adaptation Runtime:.

The adaptive runtime is implemented on the top of our DataSpaces data-management substrate [3]. DataSpaces provides distributed interaction and coordination services to support in-situ and in-transit simulation-analysis workflows, and its data transport layer provides the required asynchronous communication and data transfer services.The *Adaptation Engine* is integrated into DataSpace to enable runtime workflow coordination and adaptation at different layers. In addition, the embedded performance tools in Chombo provides runtime system information such as memory usage and execution time, and are used by the *Monitor*.

Systems:.

Our experiments were conducted on the Intrepid IBM BlueGene/P system at Argonne National Laboratory and Titan Cray-XK7 systems at Oak Ridge National Laboratory. Intrepid consists of totally 40960 nodes, each of which has 850 MHz quad-core processor and 2GB RAM (i.e., 500MB per core). Its peak performance can reach 557 teraflops.

Titan has 18,688 nodes connected through a Gemini internal interconnect, and each node has a single 16-core AMD 6200 series Opteron processor. The total system memory is 600 terabytes and the system peak performance can reach 20 petaflops.

5.2 Evaluation and Discussions

5.2.1 Evaluation of Adaptations at the Application Layer

For this experiment we used the memory intensive 3-D AMR Polytropic Gas application with a domain size of $128 \times 64 \times 64$ at base level. The experiments were performed on 4K cores of the Intrepid IBM BGP system, which has only 500MB of memory per core. Furthermore, we experimented with two different types downsampling approaches that can be used by the application layer adaptation mechanism.

User-defined range-based data downsampling: In this experiments the application layer adaptation mechanism used an in-situ user-defined down-sampling rate range. The ranges of acceptable down-sampling factors were specified as user hints, and were $\{2, 4\}$ for the first half of the simulation, and $\{2, 4, 8, 16\}$ for the second half.

In this experiment, the peak memory used on a processor varied from $20MB$ to $>$ 300MB. Figure 5 plots the online memory availability for a single processor over 40 time steps. The Figure also shows the actual memory usage during the same period when using adaptive downsampling rates, as well as the memory requirements when maximum and minimum acceptable spatial resolutions were used for the data. When sufficient memory was available (between time step 0 to 30), the adaptive mechanism correctly selected the minimum down-sampling factor, which produced a larger data volume at a higher spatial resolution. However, starting with the 31st time step, the available memory could no longer support the higher spatial resolution. As a result, the adaptive mechanism increased the downsampling factor as seen in the figure.

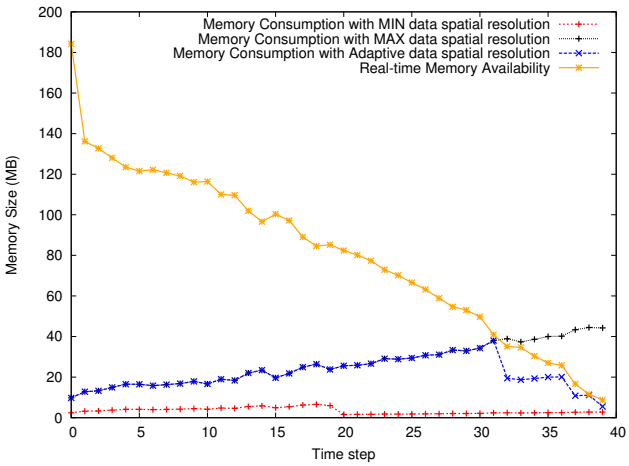


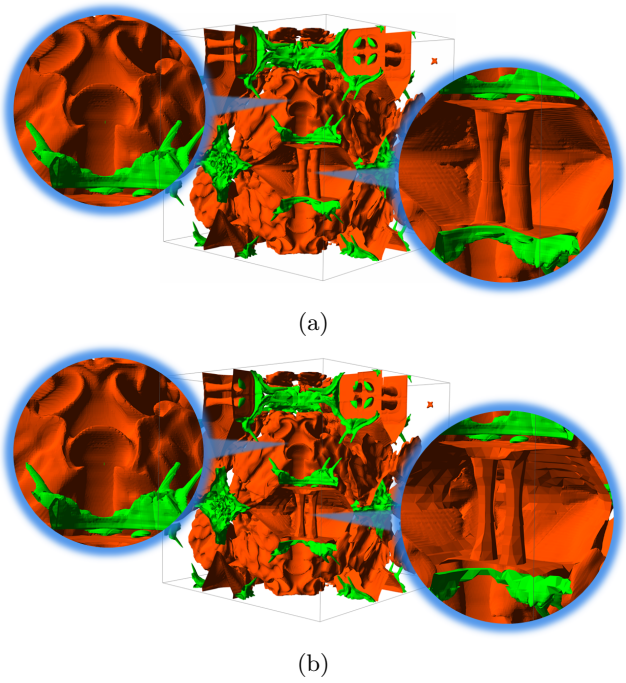
Figure 5: Evaluation of application layer adaption of the spatial resolution of the data using user-defined downsampling rates and based on runtime memory availability. At the 31st time step, the spatial data resolution is reduced due to limited availability of memory resources; and at the 40th time step, the adaptive resolution reaches the minimal value.

Entropy based data down-sampling: In this experiments, the down-sampling factors used by the application layer adaptation mechanism were automatically tuned based on information theory, which provided us with a theoretical framework to measure the information content of a variable [20]. For each data block of an AMR dataset, we compute the *entropy* value to quantify the distribution of its variables. For a discrete random variable χ and probability mass function $p(x), x \in \chi$, the entropy of X can be defined as

$$H(X) = -\sum_{x \in \chi} p(x) logp(x) \tag{11}$$

where $p(x) \in [0, 1]$, $\sum_{x \in \chi} p(x) = 1.0$, and $-logp(x)$ represents the information associated with a single occurrence of x. The higher the value of $H(x)$, the more information the data block contains. The unit of $H(X)$ is a *bit*. For example, at the 60th time step of the Polytropic Gas case, the entropy values of the data blocks at the finest level are between 5.14 and 9.85. We can now adaptively downsample the data blocks based on their entropy values by specifying a set of certain thresholds. Figure 6 compares the visualization results using the full-resolution data and the adaptively down-sampled data. We can see that the fine structural information is well preserved for the regions with the higher entropy values, while the regions with the lower entropy values can potentially be reduced aggressively without losing much information or impact our understanding of the data.

These results clearly show that our approach successfully adapts the down-sampling factor at runtime to meet the con-



(a)

(b)

Figure 6: Evaluation of application layer adaption of the spatial resolution of the data using entropy based data down-sampling. (a) shows a simultaneous rendering of two isosurfaces of the full-resolution Polytropic Gas simulation data set. The surfaces are extracted from the density variable at the 60th time step, corresponding the isovalues of 1.23 (red) and 4.18 (green), respectively. The right and left images show close up views of the two regions. (b) shows the result after the dynamic adaption of its spatial resolution. The right region has its entropy value (at 5.14) that is lower than the specified threshold and thus is down-sampled at every 4th grid point. The left region has a higher entropy value (at 9.21) and its resolution is not changed.

straints on data resolution at application layer and on the size of available memory at the resource layer. The results also show that such adaptations can potentially allow memory intensive simulation workflows to run on systems with limited available memory.

5.2.2 *Evaluation of Adaptations at the Middleware Layer*

In this experiment, we used the AMR Advection-Diffusion simulation, and evaluated both, an adaptive placement and a static placement of the visualization service within the application workflow. The experiments were performed on Titan and evaluated how middleware layer adaptations can optimize overall time-to-solution at different scales. We ran the simulation on 2K, 4K, 8K and 16K cores, with a 16:1 ratio of the number of the simulation core to the number of the in-transit cores. The initial 3D grid domain sizes were $1024 \times 1024 \times 512$ for the 2K case, $1024 \times 1024 \times 1024$ for the 4K case, $2048 \times 1024 \times 1024$ for the 8K case, and $2048 \times 2048 \times 1024$ for the 16K case.

End-to-end execution time (or time-to-solution) was the

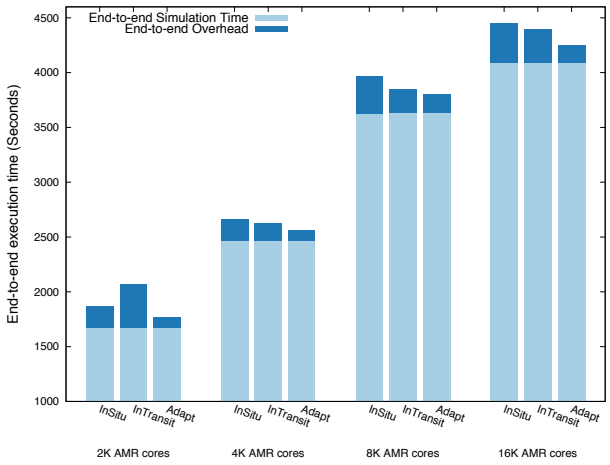


Figure 7: Comparison of cumulative end-to-end execution time between static placement (in-situ/in-transit) and adaptive placement. End-to-end overhead represents the overhead on overall time-to-solution including data processing time, data transfer time, and other system overheads.

key metric used in our evaluation and indicates how fast the users can get insights from data. The cumulative end-to-end execution time consists of two parts as seen in Figure 7: *end-to-end simulation time* and *end-to-end overhead*. End-to-end overhead represents the time cost caused by data processing, data transfers and system overheads such as adaptation. Compared with static approaches for placing analysis , our approach shows significant benefits in terms of the time-to-solution – it achieves the smallest cumulative end-to-end execution time, which matches our proposed policy that minimizes the time-to-solution by adaptive placement. Quantitatively, the cumulative end-to-end execution overhead in adaptive approach decreases by 50.00%, 50.31%, 50.50%, 56.30% compared with static in-situ placement, and 75.42%, 38.78%, 21.29%, 48.22% as compared with static in-transit placement, respectively in 2K, 4K, 8K, and 16K cases. The end-to-end overhead in all the cases are less than 6% percent of the simulation time. Meanwhile, since the analysis in some time steps are adapted to perform in-situ, the overall data movement in adaptive placement is reduced by 50.00%, 48.00%, 47.90%, 39.04% at 2K, 4K, 8K, and 16K cases, as compared to static in-transit processing placement, as shown in Figure 8.

5.2.3 *Evaluation of Adaptations at the Resource Layer*

In this experiment, we performed the local adaptations at resource layer to dynamically change the number of cores for in-transit staging. With 4,096 simulation cores, the initial number of cores available as in-transit staging resources is 256. Other configurations of this experiment are the same as those in 5.2.1. This experiment is designed to evaluate how our cross-layer adaptation respond to dynamic resource requirements to achieve an efficient CPU utilization.

Figure 9 plots results adaptation which is the number of in-transit cores for each time step. At the beginning of the simulation, the size of data generated and processed

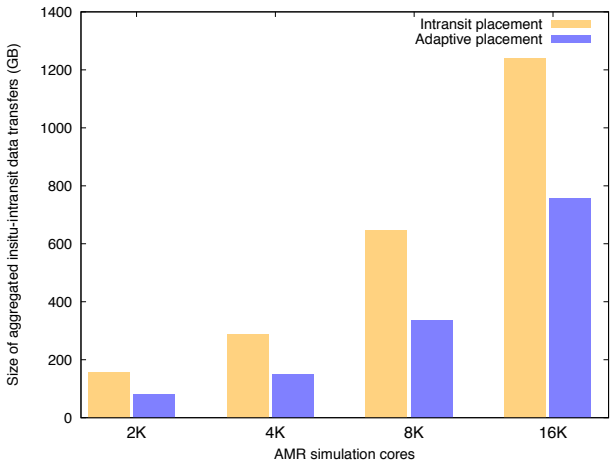


Figure 8: Comparison of total data movement with/without performing middleware adaptation.

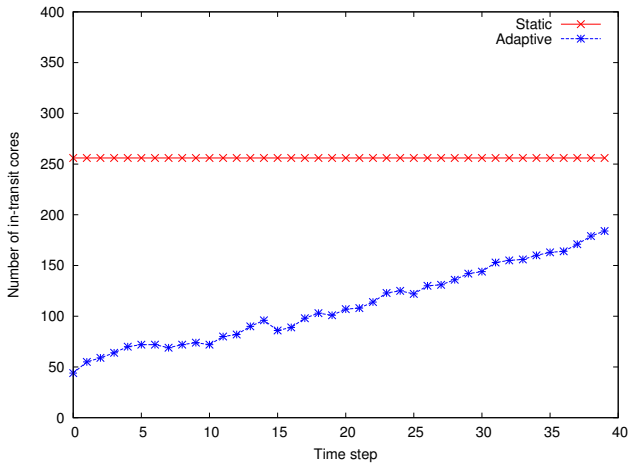


Figure 9: Number of in-transit processors when performing resource layer adaptation.

in-transit is relatively small. Therefore, only around 50 in-transit cores are needed. When the grid gets refined and more data are generated, more processors are allocated on staging area to meet the constraint of minimized time-to-solution as well as the memory resource requirement for in-transit analysis.

The adaptation approach uses fewer in-transit processor cores to achieve the same time-to-solution, compared with using a static number of in-transit cores. As a result, the resource utilization of the in-transit staging area is greatly improved. To quantify the improvement of CPU utilization, we define the cpu utilization efficiency as

$$\frac{\sum_{j=1}^{TS}\sum_{i=1}^{M_j}\{T_{intransit\_analysis\_i\_j}\}}{\sum_{j=1}^{TS}\sum_{i=1}^{M_j}\{T_{intransit\_total\_i\_j}\}} \quad (12)$$

where TS:is the maximum time step, M_j: number of in-transit cores allocated at the jth time step, $T_{intransit\_analysis\_i\_j}$: execution time of the ith in-transit processor on data analysis at the jth time step, $T_{intransit\_total\_i\_j}$: total execution time of the ith in-transit processor at the jth time step.

We find that the utilization efficiency in adaptive allocation case is 87.11%, much better than 54.57% in the case of static allocation.

5.2.4 *Evaluation of Time-to-Solution Aware Cross-layer Adaptations*

One local layer adaptation cannot meet scientists' requirements in some scenarios. For example, the scientists attempt to find the abnormities of an AMR-based simulation through visualizing the output data on the fly under a limited number of computing cores. In this case, visualizing data with lower spatial resolution is sufficient and more efficient for abnormities checking. Moreover, the visualization analysis should be adaptively performed in-situ or/and in-transit quickly and efficiently under the constraint of limited computing resources as well. We can clearly see that although application layer adaptation could adjust the data resolution adaptively, the middleware adaptation is also needed to help quickly find the abnormities. Therefore, a combined approach that can employ the adaptations on multiple layers in a coordinated manner is required.

To evaluate such global combined cross-layer adaptation on multiple layers, we ran this experiment with the objective of minimized time-to-solution. For the comparison purpose, the basic experiment workflow and settings are the same as those in experiment 5.2.2. Besides, the same acceptable user-defined data sampling rates in experiment 5.2.1 are also provided as inputs for possible application layer adaptation.

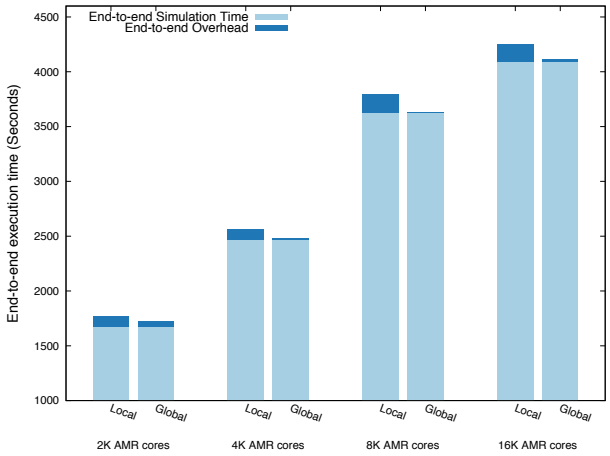


Figure 10: Comparison of cumulative end-to-end execution time between with global adaptation and with only local middleware adaptation.

The experiment result shows that all the adaptations at these three layers are employed, which matches the theoretical expectation of the global adaptation mechanism. Also, these adaptations interacted with each other. Figure 10 shows the values of overall cumulative end-to-end overhead, which decrease by 52.16%, 84.22%, 97.84%, 88.87% respectively in 2K, 4K, 8K, and 16K cases, when compared with

Cases	Total Time Steps	No. of Time Steps under Actual Utilization of In-Transit Cores			
No. of Sim Cores : No. of Staging Cores		100% Cores	75% Cores	50% Cores	Less than 50% Cores
2K:128	27	25	2	-	-
4K:256	42	8	13	4	17
8K:512	49	4	23	22	-
16K:1024	41	10	12	10	9

Table 2: Actually in-transit cores utilization while performing in-transit analysis.

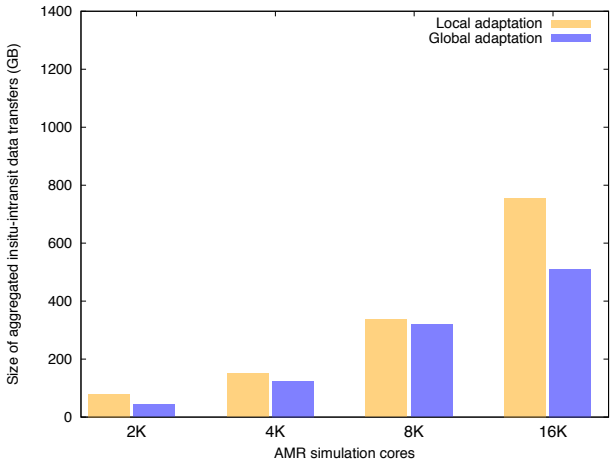


Figure 11: Comparison of total data movement between with global adaptation and with local middleware adaptation.

the results of local middleware adaptation in experiment 5.2.2. Since the raw data is adapted to be reduced in-situ, the time of both in-situ analysis and in-transit analysis decreases with the decreasing data volume. On the other hand, faster in-transit analysis means that it is more possible for staging resources to stay idle when the simulation of new time step is finished. Due to the policy of middleware adaptation, the analysis may be adapted to perform in-transit more frequently on such condition, as the results shown in Table 2.

Moreover, although performing more in-transit analysis means more data transfer, Figure 11 demonstrates that the data reduction from application layer adaptation still plays an dominant role – the overall amount of data transfer is decreased by 45.93%, 17.25%, 5.76%, and 32.41%, as compared to the results in experiment 5.2.2. Meanwhile, Table 2 shows that fewer in-transit cores are used to achieve the same time-to-solution, which demonstrates another benefit of this combined cross-layer adaptation. In 4K and 16K cases, even only less than 50% of preallocated in-transit cores are adaptively used in some of the time steps.

In summary, our cross-layer adaptation approach can be triggered and dynamically respond at runtime to meet the user-defined objectives under the varying resource limitation and user's constraints. Compared with the static approaches in other research, both the local adaptation and global combined cross-layer adaptation show benefits in terms of time-to-solution, data movement, and resource utilization efficiency. The experiment results based on Chombo-based applications and adjustable visualization code showed that our approach could be extensible to other scalable analysis approaches with no/rare communications, such as descriptive statistic analysis, data subsetting, etc.

6. RELATED WORK

Simulation-time Data Processing: The increasing performance gap between computation and I/O in high-end computing environment renders traditional post-processing data analysis approach based on disk I/O infeasible. As a result, simulation-time data processing approaches have emerged, which operate on in-memory data before it is written to file systems. Several research projects have focused on two specific simulation-time analysis techniques, namely in-situ processing and in-transit processing.

In-situ data processing allows direct access to in-memory simulation data, and has been used in visualization [14], [22], [7], indexing building [10], data compression [11], multi-physics coupling [25], etc. This technique greatly reduces the cost of data movement across network because most data is locally available in the memory. However, due to the resource sharing nature of in-situ processing, it can increase the overall time-to-solution.

In-transit data processing executes data operations on dedicated compute resources in parallel and thus minimizes the impact on main simulation and overall time-to-solution. Many projects have studied dedicated "staging" resources to support potential in-transit operations, such as DataStager [2], PreDatA [26], DataSpaces [5, 6]/ActiveSpaces [4], XpressSpace [24], GLEAN [19] and Nessie [15]. Our previous work also integrates messaging system on the staging area to support flexible data publish and subscribe [9]. However, the data movement crossing network in this approach introduces large overheads as well as power consumption.

To take advantage of both in-situ and in-transit analytic placements, many recent researches [3] have explored the benefits of combining both in-situ and in-transit approaches on leadership class supercomputers, and demonstrated the importance of where the analytics execute in a hybrid in-situ/in-transit system. FlexIO [27] exploited the trade-offs in performing analytics at different levels of the I/O hierarchy and supported a variety of simulation-analytics workloads through flexible placement options. However, these research only target static application workflows and pre-schedule the analysis placement. The adaptive analysis placement in our cross-layer adaptation framework can respond to the dynamic data management requirements of complex simulation-analysis workflows, by scheduling the placement of analysis dynamically at runtime.

Single-Layer and Cross-Layer Adaptation: Previous research efforts have focused on improving the performance by using a single-layer adaptive approach. Tapus et al. [18] introduced Resource Specification Language (RSL), a prototype language that performs the adaptation by selecting appropriate program libraries and adaptively adjusting the application parameters to tune the overall performance.

This approach only performs adaptation at the application layer and has no effect on other layers. In addition, Hsu et al. [8] proposed an algorithm that specifically targets at the hardware layer, which automatically adapts CPU settings such as voltage and frequency to reduce power consumption in HPC environment.

Meanwhile, many researchers have noticed that cross-layer adaptation could achieve performance improvement, especially when dealing with more complex workflows. For example, some cross-layer adaptation methods show encouraging results on energy saving in mobile device. Sachs et al. [17] employs a hierarchical approach that performs exhaustive global adaptation in conjunction with local adaptations. Although, at a smaller scale, they were able to achieve greater energy efficiency at four system layers: hardware layer, network layer, operating system layer, and application layer. Similarly, the GRACE-1 [23] framework was designed and implemented for mobile multimedia systems. It supports application QoS under CPU and energy constraints via coordinated adaptation in the hardware, OS, and application layers. Moreover, the idea of cross-layer has been employed in gird computing environment to deal with the problem of dynamic resource management [12].

However, the cross-layer adaptation approach has not been explored for dynamic simulation-analysis workflows. Our work proposes the cross-layer adaptation approach to enable dynamic adaptation in simulation-time data management and processing, and our large-scale experiments demonstrate the effectiveness in increasing resource efficiency and reducing overall time-to-solution on HPC system.

7. CONCLUSION AND FUTURE WORK

In this paper, we make a case for using an adaptive cross-layer approach to help coordinate data intensive simulation on large-scale systems. We focus on making run-time adaptation decisions across three different layers: application layer, middleware layer, and resource layer. We argue that adaptation is not only necessary but also vital to meet system and application's constrains. Moreover, in order to fully adapt and reap potential benefit, adaptation decisions need to be made collectively using information from all three layers as well as user's inputs.

We describe the design and system model of our cross-layer approach, which consists of three major components: a monitor, the adaptation engine, and adaptation policies. We also discuss how to realize the cross-layer adaptations and formulate the adaptation policies at each layer with corresponding triggers. Our experimental evaluation uses the AMR-based simulation codes implemented with Chombo framework and runs on both IBM BlueGene/P systems and Cray-XK7 systems. The evaluation results show the effectiveness of adaptation at each layer. Moreover, compared to the static approach, the results also show that our cross-layer approach with coordinated adaptations has better performance, in terms of reducing network data movement, improving resource utilization and minimizing time-to-solution.

Our future work includes (1) designing and formalizing corresponding programming model for such cross-layer approach to release users' programming complexity; (2) utilizing such approach on power management in dynamic simulations.

8. ACKNOWLEDGMENTS

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