A Distributed Workflow Platform for Simulation

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***Abstract*—This paper presents an approach to design, implement and deploy a simulation platform based on distributed workflows. It supports the smooth integration of existing software, e.g. Matlab, Scilab, Python, OpenFOAM, Paraview and user-defined programs. The contribution of the paper is a new feature which supports application-level fault-tolerance and exception-handling, i.e., resilience.**

Keywords-workflows; fault-tolerance; resilience; simulation; distributed systems

I. INTRODUCTION

Large-scale simulation applications are becoming standard in research laboratories and in the industry [1][2]. Because they involve a large variety of software and terabytes of data, moving around calculations and data files is not a simple process. Further, proprietary software and data often reside in locations from where they cannot be moved. Distributed computing infrastructures are therefore necessary [6][8].

This paper explores the design, implementation and use of a distributed simulation platform. It is based on a distributed workflow system and distributed computing resources. This infrastructure includes heterogeneous hardware and software components. Further, the application codes must interact in a timely, secure and effective manner. Additionally, because the coupling of remote hardware and software components are prone to run-time errors, sophisticated mechanisms are necessary to handle unexpected failures at the infrastructure and system levels. This is also critical for the coupled software that contribute to large-scale simulation applications. Consequently, specific approaches, methods and software tools are required to handle unexpected application behavior.

This paper addresses these issues. Section II is an overview of related work. Section III is a general description of a sample application, infrastructure, systems and application software. Section IV addresses resilience and asymmetric checkpointing issues. Section V gives an overview of the implementation using the YAWL workflow management system [4]. Section VI is a conclusion.

II. RELATED WORK

Simulation is nowadays a prerequisite for product design and scientific breakthroughs in most application areas ranging from pharmacy, meteo, biology to climate modeling, that all require extensive simulations and testing [6][8]. They often need large-scale experiments, including long-lasting runs, tested against petabytes volumes of data on large multi-core supercomputers [10] [11].

In such application environments, various teams usually collaborate on several projects or part of projects. Computerized tools are shared and tightly or loosely coupled. Some codes may be remotely located and non-movable. This requires distributed code and data management facilities. Unfortunately, this is prone to unexpected errors and breakdowns.

Data replication and redundant computations have been proposed to prevent from random hardware and communication failures, as well as deadline-dependent scheduling [9].

Hardware and system level fault-tolerance in specific programming environments is also proposed, e.g. Charm++ [5]. Also, middleware and distributed computing systems usually support mechanisms to handle fault-tolerance. They call upon data provenance [12], data replication, redundant code execution, task replication and job migration, e.g., ProActive [17], VGrADS [15].

However, erratic application behavior needs also to be addressed. This implies evolution of the simulation process in the event of unexpected data values or unexpected control flow. Little has been done in this area. The primary concern of the application designers and users is that of efficiency and performance. Therefore, application erratic behavior is usually handled by re-designing and re-programming pieces of code and adjusting parameter values and bounds. This usually requires the simulations to be stopped and rebuilt [15].

Departing from these solutions, a dynamic approach is presented in the following sections. It supports the evolution of the application behavior using the introduction of new exception handling rules at run-time by the users, based on occurring (and possibly unexpected) data values. The running workflows do not need to be aborted, as new rules can be added at run-time without stopping the executing workflows [13]. At worst, they need to be paused.

This allows on-the-fly management of unexpected events. It allows also a permanent evolution of the applications, supporting their continuous adaptation to the occurrence of unforeseen situations. As new situations arise

and new data values appear, new rules can be added to the workflows that will permanently be taken into account in the future. These evolutions are dynamically plugged-in to the workflows, without the need to stop the running applications. The overall application logics are therefore maintained unchanged. This guarantees a continuous adaptation to new situations without the need to redesign the existing workflows. Further, because exception-handling codes are themselves defined by new specific workflows plug-ins, the user interface to the applications remains unchanged [14].

III. APPLICATION TESTCASE

A. *Example Testcase*

An overview of a running tescase is presented here. It deals with the optimization of a car air-conditioning duct. The goal is to optimize the air flow inside the duct, maximizing the throughput and minimizing the air pressure and air speed discrepancies inside the duct. This example is provided by a car manufacturer and involves industry partners, e.g., software vendors, as well as optimization research teams (Figure 1).

The testcase is a dual faceted 2D and 3D example. Each facet involves different software for CAD modeling, e.g. CATIA and STAR-CCM+, numeric computations, e.g., Matlab and Scilab, and flow computations, e.g., Open FOAM and visualization, e.g., ParaView (Figure 1).

The testcase is deployed using the YAWL workflow management system [4]. The goal is to distribute the testcase on various partners' locations where the different software are running (Figure 2). In order to support this distributed computing approach, an open source middleware is used, namely: ProActive [17].

A first prototype was achieved using extensively the virtualization technologies (Figure 3), in particular Oracle VM VirtualBox®, formerly called Sun VirtualBox® [7]. This allowed experiments connecting virtual guest computers running heterogeneous software. These include Linux Fedora Core 12, Windows® 7 and Windows® XP on a range of local workstations and laptops (Figure 2).

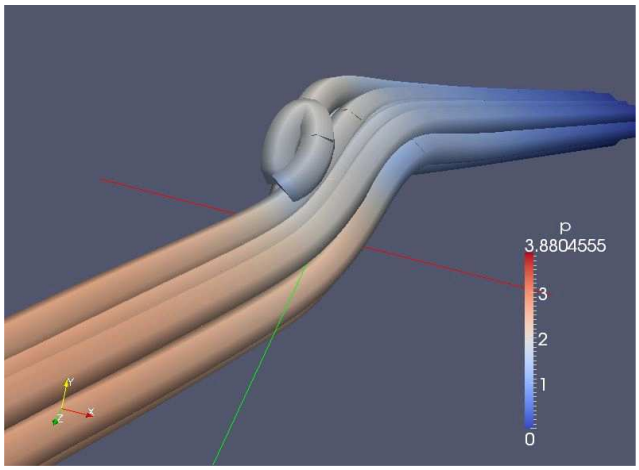

Figure 1. Pressure flow in the air-conditioning duct (ParaView display).

This work is performed for the OMD2 project, an acronym for *Optimisation Multi-Disciplinaire Distribuée*, i.e., Distributed Multi-Discipline Optimization, supported by the French National Research Agency ANR.

B. *Application Workflow*

In order to provide a simple and easy-to-use interface to the computing software, the YAWL workflow management system is used (Figure 2). It supports high-level graphic specifications for application design, deployment, execution and monitoring. It also supports the modeling of business organizations and interactions among heterogeneous software components. Indeed, the example testcase described above involves several codes written in Matlab, OpenFOAM and displayed using ParaView. The 3D testcase facet involves CAD files generated using CATIA and STAR-CCM+, flow calculations using OpenFOAM, Python scripts and visualization with ParaView. Future testcases will also require the use of the Scilab toolbox [16].

Because proprietary software are used, as well as open-source and in-house research codes, a secured network of connected computers is made available to the users, based on the ProActive middleware (Figure 5).

This network is deployed on the various partners' locations throughout France. Web servers accessed through the ssh protocol are used for the proprietary software running on dedicated servers, e.g., CATIA v5 and STAR-CCM+.

A powerful feature of the YAWL workflow system is that composite workflows can be defined hierarchically [4]. They can invoke external software, i.e., pieces of code written in whatever language is used by the users. They are called by custom YAWL services or local shell scripts. Web Services can also be invoked. Although custom services need Java classes to be implemented, all these features are natively supported in YAWL.

YAWL thus provides an abstraction layer that helps users design complex applications that may involve a large number of distributed components (Figure 3). Further, the workflow specifications allow alternative execution paths which may be chosen automatically or manually, depending on data values, as well as parallel branches, conditional branching and loops. Also, multiple instance tasks can execute in parallel for different data values. Combined with the run-time addition of code using the corresponding dynamic selection procedures, as well as new exception handling procedures (see Section IV), a very powerful environment is provided to the users [4].

IV. RESILIENCE

A. *Fault-tolerance*

The fault-tolerance mechanism provided by the underlying middleware copes with job and communication failures. Job failures or time-outs are handled by reassignment of computing resources and re-execution and of the jobs. Communication failures are handled by re-sending appropriate messages. Thus, hardware breakdowns are handled by re-assigning running jobs to other resources,

which imply possible data movements to the corresponding resources. This is standard for most middleware [17].

B. Resilience

Resilience is commonly defined as "the ability to bounce back from tragedy" and as "resourcefulness" [18]. It is defined here as the ability for the applications to handle correctly unexpected run-time situations, possibly – but not necessarily – with the help of the users.

Usually, hardware, communication and software failures are handled using hard-coded fault-tolerance software [15]. This is the case for communication software and for middleware that take into account possible computer and network breakdowns at run-time. These mechanisms use for example data and packet replication and duplicate code execution to cope with these situations [5].

However, when unexpected situations occur at run-time, which are due to unexpected data values and application erratic behavior, very few options are offered to the users: ignore them or abort the execution, analyze the errors and later modify and restart the applications.

Optimized approaches can be implemented in such cases trying to reduce the amount of computations to be re-run, or anticipating potential discrepancies by multiplying some critical instances of the same computations. This latter approach can rely on statistical estimations of failures. Another approach for anticipation is to prevent total loss of computations by duplicating the calculations that are running on presumably failing nodes [9].

While these approaches deal with hardware and system failures, they do not cope with application failures. These can originate from:

- Incorrect or incomplete specifications.
- Incorrect or hazardous programming.
- Incorrect anticipation of data behavior, e.g., out-of-bounds data values.
- Incorrect constraint definitions, e.g., approximate boundary conditions.

To cope with this aspect of failures, we introduce an application-level fault management that we call *resilience*. It provides the ability for the applications to survive, i.e., to restart, in spite of their erroneous prevailing state. In such cases, new handling codes can be introduced dynamically by the users in the form of specific new component workflows.

This requires a roll-back to a consistent state that is defined by the users at critical checkpoints.

In order to do this efficiently, a mechanism is implemented to reduce the number of necessary checkpoints. It is based on user-defined rules. Indeed, the application designers and users are the only ones to have the expertise required to define appropriate corrective actions and characterize the critical checkpoints. No automatic mechanisms can be substituted for them, as is the case in hardware and system failures. It is generally not necessary to introduce checkpoints systematically, but only at specific locations of the application processes, e.g., only before parallel branches of the applications. We call this approach *asymmetric checkpoints*. This is described in Section D, below.

C. Exception Handling

The alternative used proposed here to cope with unexpected situation is based on the dynamic selection and exception handling mechanism featured by YAWL [13].

It provides the users with the ability to add at run-time new rules governing the application behavior and new pieces of code that will take care of the new situations.

For example, it allows for the runtime selection of alternative workflows, called worklets, based on the current (and possibly unexpected) data values. The application can therefore evolve over time without being stopped. It can also cope later with the new situations without being altered. This refinement process is therefore lasting over time and the obsolescence of the original workflows reduced.

The new worklets are defined and inserted in the original application workflow using the standard specification approach used by YAWL (Figure 2).

Because it is important that monitoring long-running applications be closely controlled by the users, this dynamic selection and exception handling mechanism also requires a user-defined probing mechanism that provides with the ability to suspend, evolve and restart the code dynamically.

For example, if the output pressure of an air-conditioning pipe is clearly off limits during a simulation run, the user must be able to suspend it as soon as he is aware of that situation. He can then take corrective actions, e.g., suspending the simulation, modifying some parameters or value ranges and restarting the process immediately. These actions can be recorded as new execution rules, stored as additional process description and invoked automatically in the future.

These features are used to implement the applications erratic behavior manager. This one is invoked by the users to restart the applications at the closest checkpoints after corrective actions have been manually performed, if necessary, e.g., modifying boundary conditions for some parameters. Because they have been defined by the users at critical locations in the workflows, the checkpoints can be later chosen automatically among the available asymmetric checkpoints available that are closest to the failure location in the workflow.

D. Asymmetric Checkpoints

Asymmetric checkpoints are defined by the users at critical execution locations in the application workflows. They are used to avoid the systematic insertion of checkpoints at all potential failure points. They are user-defined at specific locations, depending only on the application logic. Clearly, the applications designers and users are the only ones that have the domain expertise necessary to insert appropriately these checkpoints. In contrast with middleware fault-tolerance which can re-submit jobs and resend data packets, no automatic procedure can be implemented here. It is therefore based on a dynamically evolving set of heuristic rules.

This approach significantly reduces the number of necessary checkpoints to better concentrate on only those that have an impact on the applications runs [3].

For example (Figure 4):

- The checkpoints can be chosen by the users among those that follow long-running components and large data transfers.
- Alternatively, those that precede sequences of small components executions.

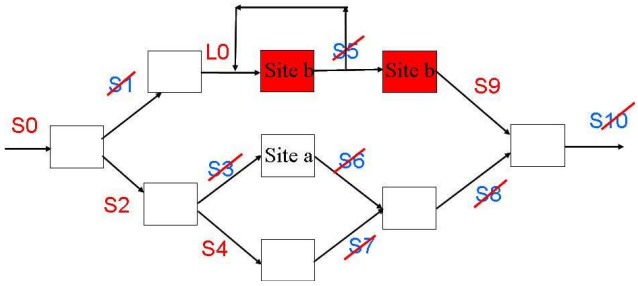

Figure 4. Asymmetric checkpoints example.

The basic rule set on which the asymmetric checkpoints are characterized is the following:

- R1: no output backup for specified join operations.
- R2: only one output backup for fork operations.
- R3: no intermediate result backup for user-specified sequences of operations.
- R4: no backup for user-specified local operations.
- R5: systematic backup for remote inputs.

This rule set can be evolved by the user dynamically, at any time during the application life-time, depending on the specific application requirements. This uses the native rule mechanism in YAWL [13].

V. IMPLEMENTATION

A. *Resilience*

Resilience is the ability for applications to handle unexpected behavior, e.g., erratic computations, abnormal result values, etc. It is inherent to the applications logic and programming. It is therefore different from systems or hardware errors and failures. The usual fault-tolerance mechanisms are therefore inappropriate here. They only cope with late symptoms, at best.

New mechanisms are therefore required to handle logic discrepancies in the applications, most of which are only discovered incrementally during the applications life-time, whatever projected exhaustive details are included at the application design time.

It is therefore important to provide the users with powerful monitoring features and to complement them with dynamic tools to evolve the applications specifications and behavior according to the future erratic behavior that will be observed during the application life-time.

This is supported here using the YAWL workflow system so-called “dynamic selection and exception handling mechanism” [4]. It supports:

- Application update using dynamically added rules specifying new worklets to be executed, based on data values and constraints.
- The persistence of these new rules to allow applications to handle correctly the future occurrences of the new cases.
- The dynamic extension of these sets of rules.
- The definition of the new worklets to be executed, using the native framework provided by the YAWL specification editor: the new worklets are new component workflows attached to the global composite application workflows [13].
- Worklets can invoke external programs written in any programming language through shell scripts, custom service invocations and Web Services [14].

B. *Distributed workflows*

The distributed workflows rely on the interface between the YAWL engine and the ProActive middleware (Figure 5). Users provide a specification of the simulation applications using the YAWL Editor. It supports a high-level abstract description of the simulation processes (Figure 2).

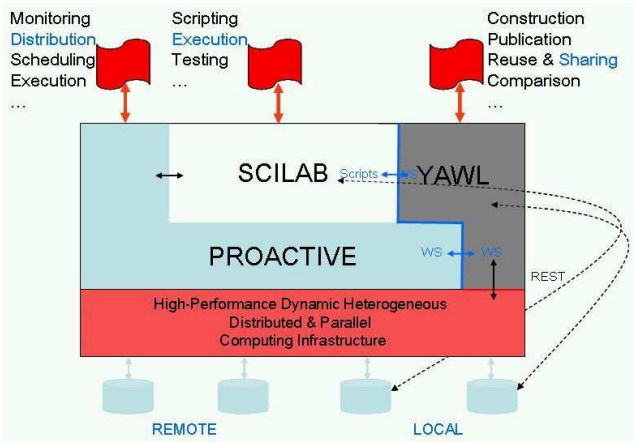

Figure 5. The OMD2 distributed simulation platform.

These processes are decomposed into components which can be other workflows or basic workitems. The basic workitems invoke executable tasks, e.g., shell scripts or so-called “custom services”. These custom services are specific execution units that call user-defined YAWL services. They support interactions with external and remote codes. In this particular platform, the remote external services are invoked through the ProActive middleware interface (Figure 6).

This interface delegates the distributed execution of the remote tasks to the ProActive middleware [17]. The middleware is in charge of the distributed resources allocation to the individual jobs, their scheduling, and the coordinated execution and result gathering of the individual tasks composing the jobs. The scheduler default policy is “best-effort”. However, users can implement their own policy, if desired. The middleware also takes in charge the fault-tolerance related to hardware, communications and system failures. The resilience, i.e., the application-level fault-tolerance is handled using the rules described in the previous sections.

The remote executions invoke the middleware functionalities through ProActive's Java API. The various modules invoked are the ProActive Scheduler, the Jobs definition module and the Tasks which compose the jobs. The jobs are allocated to the distributed computing resources based upon the scheduler policy. The tasks are dispatched based on the job scheduling and resource allocation. They invoke Java executables, possibly wrapping code written in other programming languages, e.g., Matlab, Scilab, Python, or calling other software, e.g., CATIA v5, STAR-CCM+, ParaView, etc.

Optionally, the workflow can invoke local tasks using shell scripts and remote tasks using Web Services. These options are standard in YAWL [4]. Calling the ProActive middleware is however necessary to run tasks on large multi-core clusters. ProActive is here in charge of the scheduling and resource allocation in these highly parallel environments, which YAWL does not support natively.

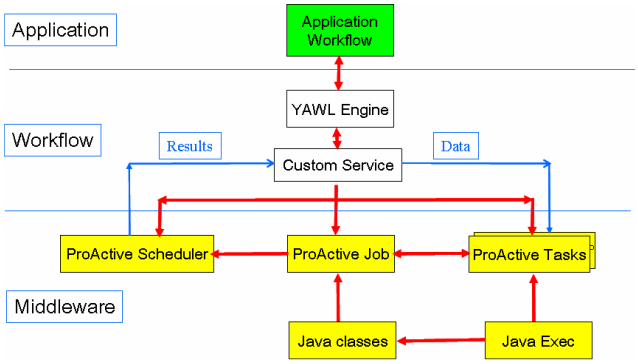

Figure 6. The YAWL workflow / ProActive middleware interface.

VI. CONCLUSION

The requirements for large-scale simulations make it necessary to deploy various software components on heterogeneous distributed computing infrastructures. These environments are often required to be distributed among a number of project partners for administrative and organizational purposes.

This paper presents an experiment for deploying a distributed simulation platform. It uses a network of high-performance computers connected by a middleware layer. Users interact dynamically with the applications using a distributed workflow system. It allows them to define, deploy and control the application executions.

A significant bonus of this approach is that besides fault-tolerance provided by the middleware, which handles communication, hardware and system failures, the users can define and handle the application failures at the workflow specification level.

This means that a new abstraction layer is introduced to cope with the application errors at run-time. Indeed, these errors do not necessarily result from programming and design errors. They may also result from unforeseen situations, data values and boundary conditions that could not be envisaged at first. This is often the case in simulations due to the experimental nature of the applications, e.g., discovering the behavior of the system being simulated, like unusual flight dynamics: characterization of the stall behavior of an aircraft for various load and balance profiles [2].

This provides support to resilience using an asymmetric checkpoints mechanism. This feature allows for efficient handling mechanisms to restart only those parts of an application that are characterized by the users as critical for overcoming erratic behavior.

Further, this approach can evolve dynamically, i.e., when applications are running. This uses the native dynamic selection and exception handling mechanism in the YAWL workflow system [4]. Should unexpected situations occur, it allows for new rules and new exception handlers to be plugged-in at run-time.

New testcases are currently being designed that involve large-scale (1000 CPU hours) simulations, e.g., car aerodynamics, running on a network of multi-core clusters.

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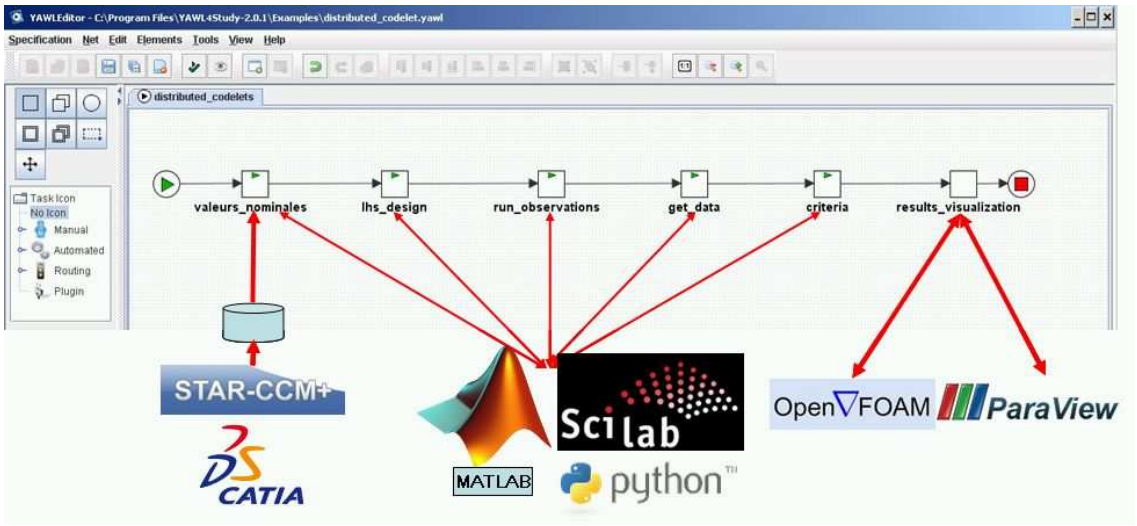

Figure 2. The YAWL workflow interface for the 2D testcase.

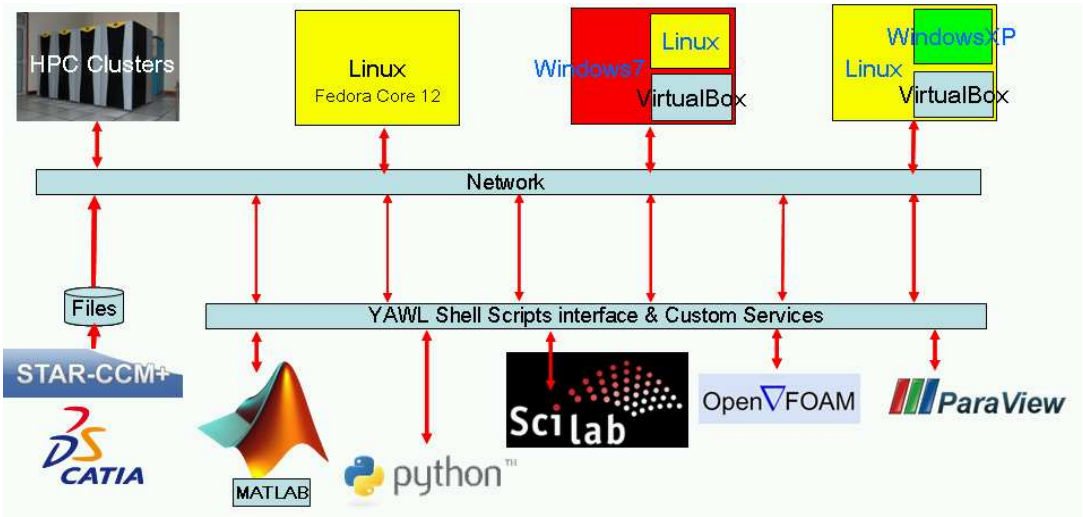

Figure 3. The virtualized distributed infrastructure.