TOWARDS AN ERROR DETECTION TEST FRAMEWORK FOR MOLECULAR DYNAMICS APPLICATIONS

By

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ABSTRACT OF THE THESIS

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The reliability of a fully developed software is critical, since it determines a software's credibility and user satisfaction in the application. A major challenge in the field of testing is to bridge the gap between the customer requirements and the actual outcome of the software. There are several applications in the field of chemical sciences for Molecular Dynamics (MD) simulations. These applications are chemical engineers' tools to study the simulations and analyze the results. The EnsembleMD Toolkit and RepEx are Python-based tools for developing MD applications providing an abstraction that enables the efficient and dynamic usage of High Performance Computing (HPC).

The EnsembleMD toolkit and RepEx facilitates a simple framework for MD applications, but they lack the feature of testing their functionality during Software Development Life Cycle (SDLC). Checking the errors and faults at all stages of the SDLC, namely, development, deployment and run-time is crucial to ensure the proper functioning of the scientific tools and applications.

Frequent changes in the system configuration of supercomputers impose the necessity of a platform which can provide a sanity check on all the components. To address these requirements, we have developed a Testing Framework. This framework has three primary design components: (1) Support of testing the Application Program Interfaces (APIs) of the toolkit during development, (2) Support for testing of faults during their deployment on supercomputers and (3) Support for logging the run-time exceptions and errors. This test bench enables the developers of various scientific tools viz. EnsembleMD, RepEx, Amber, etc. to easily and scalably debug the issues faced by the users.

Acknowledgments

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Dedication

Dedicated to family and friends

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Chapter 1
Introduction

1.1 Motivation

As supercomputers and HPC clusters increase in size and complexity, system failures have become inevitable [7]. These failures have a great impact on the available computing resources. Around 1.53% of the total applications failed during the initial 518 production days of the Blue Waters supercomputer contributing to 9% of the total production node hours [6]. These failures are reported not only because of the system errors, but might also occur due to an application or software bug. A software bug is an error in the programming and coding of an application that might cause it to malfunction. These bugs often have a major impact on cost, money and time. Software failures can lead to serious consequences both in safety critical and normal applications. Software testing is defined as a formal process in which a software unit, several integrated software units, or an entire package, is examined by running the programs on a computer with various inputs and expected outputs. It is the primary method for assuring high quality and error free software. All the associated tests are expected to generate results similar to the results generated during actual execution. Software testing plays a central role in the quality assurance of any application. In SDLC, testing is paramount during the development and pre-delivery phases of any software.

A testing framework is essential for error control that can be categorized into error detection and error handling and correction. Error detection is the most important stage for developing reliable and highly dependable computing as it deals with the detection of errors generated due to software defects or hardware failures. The error report generated by the error detection phase can be used by the developers to handle and rectify the defects. Testing is a continuous cycle of error control mechanisms which operates until the software has negligible defects or the errors lie within the acceptance criteria. A plethora of applications has been developed to perform MD simulations and analysis. Many of these applications in the field of molecular sciences use ensemble-based methods as their basis to make scientific progress. EnsembleMD toolkit is one such toolkit that provides an abstraction layer for executing various scientific simulations where multiple computational execution units form a part of an ensemble referred to as *tasks.*

Traditionally, developers of the EnsembleMD toolkit had to back trace all the logs from supercomputers, logs from RADICAL-Pilot and EnsembleMD to debug any failures or exception issues. Job submission and execution on remote supercomputers may fail due to various factors, viz. failure due to bugs in source code, wrong kernel inputs, exception if the connection to database fails, failed job submission or if the modules and configurations specific to the kernel and supercomputer are loaded incorrectly. A large number of logs generally lead to multiple drawbacks. The major drawback is to isolate the error and exception causing components. It is cumbersome to debug innumerable logs and investigate the failures and faults. The failures and errors in the software can also be reported by the users using different hardware or compilers. Inefficient testing on all of the platforms can cause a loss of developers' precious time and efforts to identify and isolate these errors [13]. As discussed earlier, detecting errors is crucial in error control mechanism of any test framework, the aforementioned problem to detect errors in MD applications serves as the motivation for this thesis. The developers and the users of EnsembleMD toolkit and other scientific toolkits would benefit largely from this testing framework that encapsulates the following:

- Automate the cumbersome process of debugging and isolating errors and exceptions.
- Support a test bench to ensure the expected functionality of all of the APIs in the toolkit.
- Eliminate manual efforts to check for proper configurations required by supercomputers to execute different kernels.
- Possess the capability to execute all of the tests automatically whenever functionality of the toolkit is added or modified.

1.2 Objective

The main objective of this thesis is to develop a test framework to enable the validation of open source tools like the EnsembleMD toolkit and RepEx and to test the proper functioning of all of the APIs. Furthermore, the aim is also to develop a framework that tests the deployment and runtime errors which may occur while executing scientific tools on remote supercomputers. Another objective is to analyze the requirements and develop an automated test bench for the developers with the following capabilities:

- Enable a test bench to ensure that the development code meets its design requirements.
- Enable remote supercomputer configuration and environment checking at the time of deployment.

- Enable a framework to detect the run-time faults and errors by mining the logs generated on the supercomputers at the time of execution of an application.
- Ensure that the toolkit behaves as expected and provides interoperability to enable execution over multiple heterogeneous distributed computing infrastructure.

1.3 Structure of the Thesis

After discussing the motivation and objectives for this thesis in Chapter 1, we will discuss the various research and related works in Chapter 2 followed by a discussion on the background of the RADICAL EnsembleMD toolkit and RADICAL RepEx framework in Chapter 3. In Chapter 4, we will explore the testing infrastructure, its significance and testing framework design for the toolkits. In Chapter 5, we will discuss the development level testing of EnsembleMD and RepEx. Development level testing includes unit testing and end-to-end testing to ensure a bug-free tool. SATLite, a standalone testing tool to test deployment and run-time errors will be discussed in Chapter 6. Chapter 7 illustrates the automated testing harness and integration with the Jenkins Continuous Integration (CI) server in depth along with the testing results. In Chapter 8, we arrive at the conclusion and discuss the foundations this thesis lays for future work.

Chapter 2
Related Work

A large percentage of today's HPC efficiency and resources are wasted due to various failures. These failures significantly affect the capacity of HPC clusters. These may occur due to either HPC system failures or the application level failures. The logs generated by the clusters are abundant and mining these logs to detect the error is very cumbersome.

Existing research work investigates system diagnostic logs and primarily focuses on detecting the faults generated with HPC system as a frame of reference. A large number of mining tools have been developed to study and analyze these logs. Martino et al. [6] studied the impact of system failures on Blue Waters. Their study emphasized the effect of these failures on the available node hours. To study and analyze these failures, they have developed *LogDiver* which is a tool to automate the system log data processing. *LogDiver* handles a large amount of textual data extracted from the system and application level logs and decodes the specific types of events and exit codes. They have shown that the failing applications contribute to 9% of the total node hours affecting the system resources. Their study also shows that probability of application failures due to HPC system failures is just 0.162. The detection of errors and failures at the application level is, therefore, inevitable and testing the faults with the application as a frame of reference is equally important.

The current ongoing research primarily focuses on providing fault tolerance strategies with an objective to minimize the fault and failure effects on supercomputer resources. These studies show how to combat the effect of system failures and predict them to minimize the errors and faults. Chuah et al. [9] studied the root causes of the failures using system logs of the Ranger supercomputer at the Texas Advanced Computing Center (TACC). *FDig*, a diagnostic tool had been developed to extract the log entries as structured message templates to analyze the faults. *FDig* detects the frequency of the specific errors by extracting the error template messages from the stored system logs and supports system administrators in the fault diagnostic processes.

Gainaru et al. [10] extensively exploited the concepts of data mining techniques to determine system errors from the logs generated by Blue Gene/L machine. According to Papers [6], [8], [9], [11], console logs are a primary source of information about the condition of a cluster or HPC system. These error logs help system administrators to analyze the causes of system failures.

A study by Oliner et al. [12] on the system logs from five supercomputers, namely, Blue Gene/L, Red Storm, Thunderbird, Spirit and Liberty which analyzed failure alerts and actual failure, shows that a large number of alerts are generated due to hardware issues, but most of the system failures are due to software issues. A possible explanation for system failure may also be due to software upgrades. The applications running on these resources might not be compatible with the software upgrades and hence leading to their failure. Our thesis is also capable of detecting the application failure due to HPC system upgrades.

All of the novel approaches discussed earlier in this section describes the strategies to anatomize the system logs and error log files to detect the system errors. These techniques make use of past logs to predict the plausible causes of failure. There is a window of opportunity for further improvement in the efficiency of supercomputer resources if we can minimize the errors during application job submission and faults occurring at the application level. The large sector of computing resources is used by MD simulations. These applications are responsible for complex simulation and analysis of various molecular structures. There is always a major cost associated if these MD applications fail. The scientific simulation workflows such as Amber, CoCo, etc. are the major tools in the field of the MD domain. These workflows serve as input to various tools such as RADICAL EnsembleMD [23] and RepEx [24]. With the advancement in these workflows, it is highly possible to have software bugs. In order to minimize the effect of application failures due to source code bugs, improper environment loading or transferring incorrect input files, we have developed a testing tool, *Simple Application Testing Lite (SATLite)* to detect the application deployment level and run-time errors. As discussed earlier, SATLite also uses log mining approach to detect faults and exceptions. As discussed in Paper [6], failed applications contribute majorly towards the wastage of supercomputer resources, SATLite aims at minimizing these failures before distributing the application to the end user, and thus saving a large number of node hours.

The developers of scientific workflows can directly check for errors while their software is still under development, before releasing it to their user base. The dependency of these scientific simulation packages on different operating systems and HPC clusters remains undetected unless a full compilation is made, and errors with"make clean" [13] can build successfully on a developer's machine, but can fail on user machines. Betz et al. [13] have discussed the effect of application bugs with respect to Amber development in depth. Since major research in the field of HPC fault-tolerance system uses logs to predict or combat the failures at the supercomputer end, we make use of these logs with an aim to detect the application failures both due to supercomputer issues and providing unit testing results for RADICAL tools.

pyPcazip [28] is a Python-based analysis tool for MD simulation data similar to RADICAL

EnsembleMD and RepEx. pyPcazip has a testing suite that tests all the APIs with different inputs on different HPC clusters. A similar test framework has been implemented for Mist [29], a C++ library for the MD simulations. The test framework developed for Mist generates a test report for each testing cycle, providing developers a detailed analysis of all the software bugs and failures. RADICAL Pilot [25] serves as the basic layer for EnsembleMD toolkit and Repex. RADICAL Pilot has a fully developed functional test [27] framework to test all of its components and it is able to capture most of the software bugs. We have designed the testing framework for EnsembleMD toolkit and RepEx on the similar tracks separating each iteration of tests in different report folders based on date and time. Also, different parts of the API tests can be invoked independently. The study of different test frameworks and their implementation provided a background for developing a testing framework for RADICAL EnsembleMD and RADICAL Pilot. Using the available research, this thesis accommodates log mining based fault detection approach from MD application's perspective and provides unit testing results of RADICAL EnsembleMD and RepEx to aid RADICAL developers with a motivation to optimize the use of HPC resources.

Chapter 3
Background of RADICAL Tools

MD simulation is a key method to study protein structures, gene finding, sequence analysis etc. These simulations are highly important in the field of drug design and drug discovery to study active molecules and protein interaction sites [1]. The gene sequence and protein structures are highly important in the detection of diseases, hence, the analysis of these components is highly critical and requires high computing. Due to the high complexity of the molecule structure, high performance and parallel computing provide a substantial improvement in the time taken for various calculations. The HPC approach helps to minimize the number of target drugs that are required to be tested by expensive and time-consuming synthesis and laboratory experiments [1]. There are several tools that provide an interface for the MD simulations. ExTASY tools such as Amber, CoCo, Gromacs and LSDMap are the scientific tools for MD simulations. RADICAL-EnsembleMD toolkit (EnMDTK) and RepEx provides an interface for the resource handling and execution of the former tools on the remote HPC clusters. This chapter deals with the background discussion of the toolkit whose testing framework has been developed.

3.1 About the EnsembleMD Toolkit

EnsembleMD Toolkit is a Python-based framework for developing, simulating and executing molecular science applications comprising ensembles of simulations. This toolkit is designed to address the issues of decoupling of tasks, heterogeneity across them and the dependency between them [3], [23]. This provides a tool for MD applications which efficiently decouples the details of execution units and manages their submission on the remote machines. It provides an abstraction to the users, hiding the complexity of the mechanism of job submission, execution and data transfer. The EnsembleMD toolkit provides a set of explicit, predefined patterns, that are found in ensemble-based MD workflows [2], [3], [23]. Users have an advantage of picking up the patterns which represent their application and populate it with MD engines viz. Amber, Coco, Gromacs or LSDmap, represented by 'kernel' in the tool. Even though traditional tools gave complete control to users to manage MD applications, the major drawback was that the user was required to have knowledge of load transfer,

job submission or data flow control. Users were required to explicitly undergo these cumbersome tasks of resource allocation, job submission and execution. In the case of the EnsembleMD toolkit, this complexity is hidden from the user, hence it provides a simple yet efficient way to execute their application.

3.1.1 Design of EnsembleMD Toolkit

Ensemble-based applications comprise tasks that may vary in the type of coupling between them or the amount of information transferred between them. Each of the tasks, with or without coupling, have different computational requirements [2], [3]. The EnsembleMD toolkit was designed with an aim to provide a framework for multiple tasks with varying coupling levels on different HPC clusters. The modular design of the tool serves as a building block to make MD application execution flexible and scalable.

Figure 3.1 [23] shows the architecture of EnsembleMD toolkit. As depicted in the figure, execution of any MD application takes place in five steps, namely:

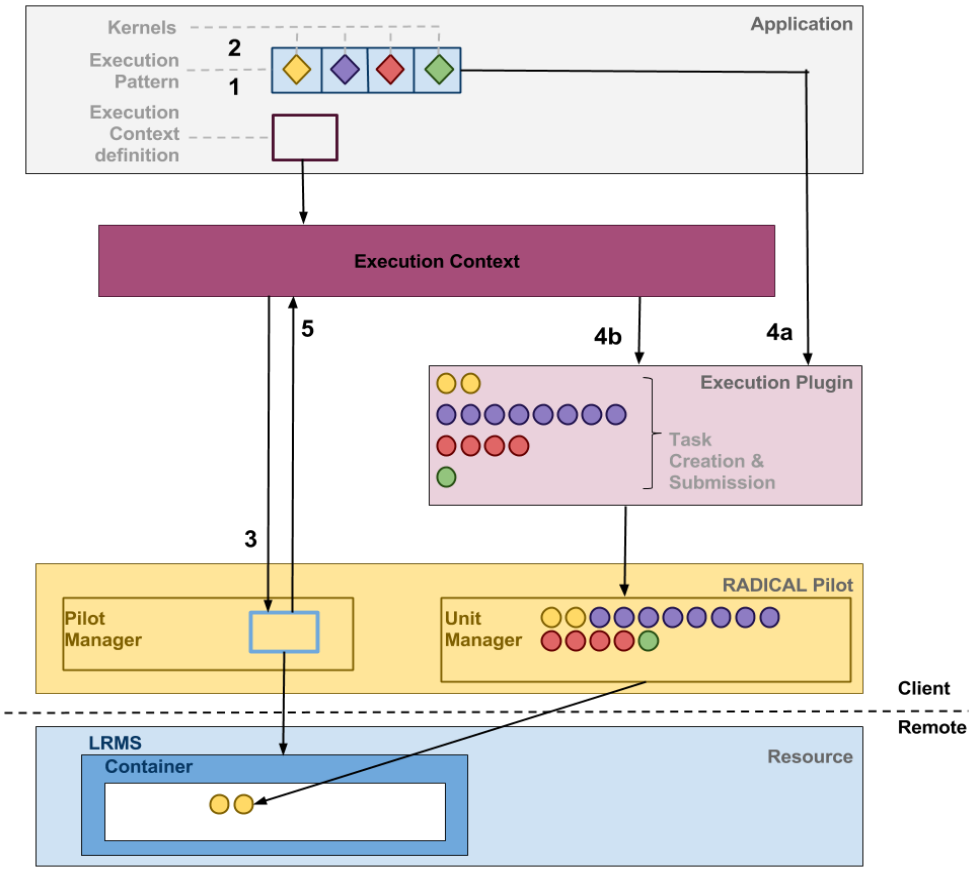
- Pick execution pattern representing the application.
- Define kernel plug-in for various stages of the pattern.
- Resource handler creation and request for resource submission.
- Call Execution plug-in to bind pattern and kernel plug-in and run the job on the remote resource.
- After successful execution, de-allocate the resources and user gets back the control.

3.2 EnsembleMD Toolkit Components

As discussed in the above steps, the EnsembleMD tool architecture comprises of four basic components showcasing the heterogeneous property of the tool that is described in details in subsequent subsections.

3.2.1 Execution Patterns

MD application control flow can be categorized into a few repeating types. The EnsembleMD tool exploits this characteristic to define a high-level object describing the control flow or *"what to do"* at different stages. An execution pattern represented by **1** in figure 3.1 describes a parameterized container which can hold and execute ensembles.



Credit: EnsembleMD toolkit architecture document [23]

Figure 3.1: Architecture of EnsembleMD Tool

3.2.2 Kernel Plugins

A Kernel plug-in represented by **2** in figure 3.1 is an object that performs a computational task in this toolkit. It represents the instantiating of a specific science tool along with the required software environment. Kernel hides tool-specific peculiarities across different clusters as well as differences between the interfaces of the various MD tools to the extent possible.

3.2.3 Resource Handler

The resource handler represented by **3** in figure 3.1 manages the resources for various job submission and execution on HPC cluster. It provides the following methods:

- Allocate resource
- Run execution pattern on allocated resource
- De-allocate resource

3.2.4 Execution Plug-in

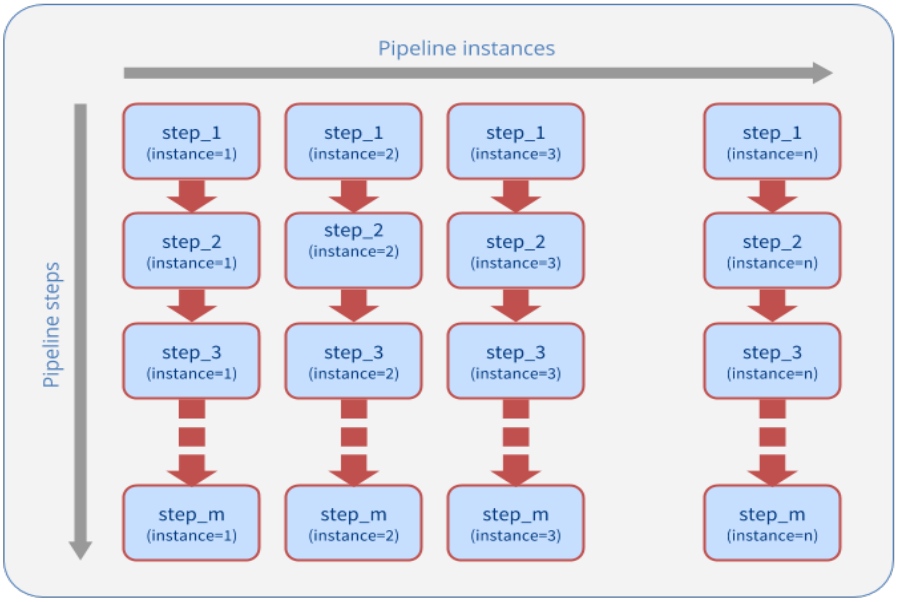
The execution plug-in represented by **4** in figure 3.1 is an internal component of the toolkit managing the execution of the execution patterns. This layer binds the execution pattern with the kernel plug-ins, hence, generating the executable units which are forwarded to the underlying run-time system along with the resource details. This plug-in decouples the execution plug-in into an executable plug-in enhancing the run-time optimization of various parameters, viz. time to completion, throughput etc. As we have discussed earlier, the EnsembleMD toolkit is an abstraction tool which hides the complexity within the underlying layers and only exposes the plug-ins to the users. Execution pattern, kernel plug-in and resource handlers are exposed to the users, whereas the execution plug-in manages the underlying complexity of decoupling the tasks, binding patterns and plug-ins, job submission, job execution and data transfer. This hidden complexity is addressed by the RADICAL-Pilot layer, which is the most crucial component of the toolkit architecture.

3.2.5 RADICAL Pilot

RADICAL-Pilot is a Pilot job framework which allows users to run many computational tasks simultaneously on one or more different distributed systems such as remote HPC clusters. A Pilot-job is responsible for acquiring resources necessary to execute the computational units on the HPC cluster. The Pilot-job submits the jobs or the units to the system's batch queue. These pilot jobs are the containers that carry the number of tasks or executable within itself. Once these pilot jobs become active, it can run sub-jobs directly, by eliminating the need to submit a separate job for each executable differently and hence, reducing time-to-completion. RADICAL Pilot provides task-level parallelism, by executing a large number of tasks concurrently on the HPC cluster. In other words, typically in the absence of any such job submission framework, if the application has a complex work flow that requires several tasks to be executed, each task or job is required to be submitted individually with the queue wait time. This call for a resource management framework can effectively submit parallel jobs, hence, enhancing the effective use of the available resources.

3.3 Patterns in EnsembleMD Toolkit

As discussed earlier, the workflows in molecular sciences applications can be categorized into repeating types, motivating the developers to create an abstraction layer called "patterns." EnsembleMD toolkit has four patterns which envelopes almost all the MD applications. The next few subsections will discuss the different types of "patterns."



Credit: EnsembleMD toolkit architecture document [23]

Figure 3.2: Pipeline Pattern

3.3.1 Pipeline

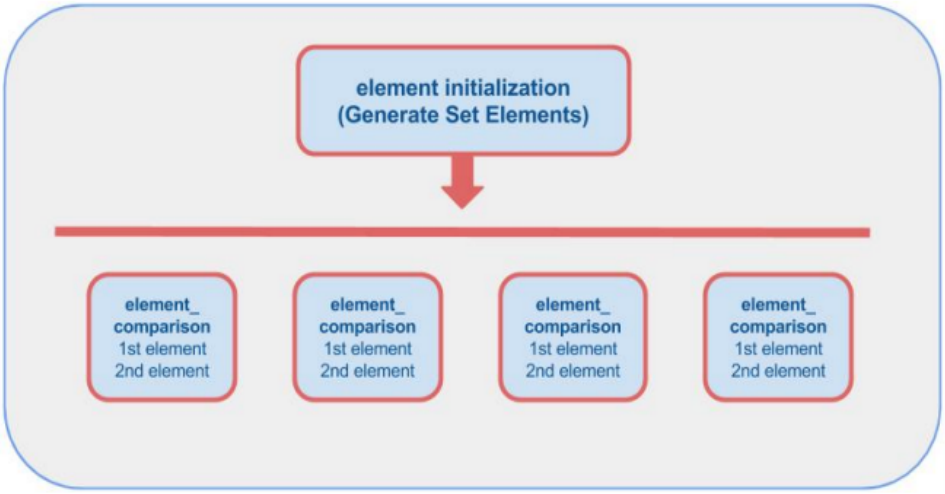
A pipeline pattern consists of a sequence of executable stages. The EnsembleMD toolkit pipeline pattern, as shown in Figure 3.2 [23], is the primary pattern that consists of a container of independent tasks that contains heterogeneous workloads. The data flow and control mechanism is always unidirectional and follows a linear pattern. Each pipeline stage might have a dependency from the previous stage and executes independently.

3.3.2 AllPairs

The All-pairs problem is stated as: All-Pairs(set A, set B, function F) returns a matrix M which is composed by comparing all elements of set A to all elements of set B using the function F. Otherwise stated as, M[i,j] = F(A[i],B[j])[12]. A pictorial representation is given in Figure 3.3.

3.3.3 Replica Exchange

Replica Exchange pattern is a generalization of Replica Exchange Molecular Dynamics (REMD) conformational algorithm [4] and is divided into two stages, namely: Simulation stage and Execution stage. The Replica Exchange pattern starts with each replica propagating to simulation phase independently, followed by the exchange phase where an exchange of thermodynamic patterns takes place. This exchange is determined on the basis of the results of the simulation phase. Figure 3.4



Credit: EnsembleMD toolkit architecture document [23]

Figure 3.3: Allpairs Pattern

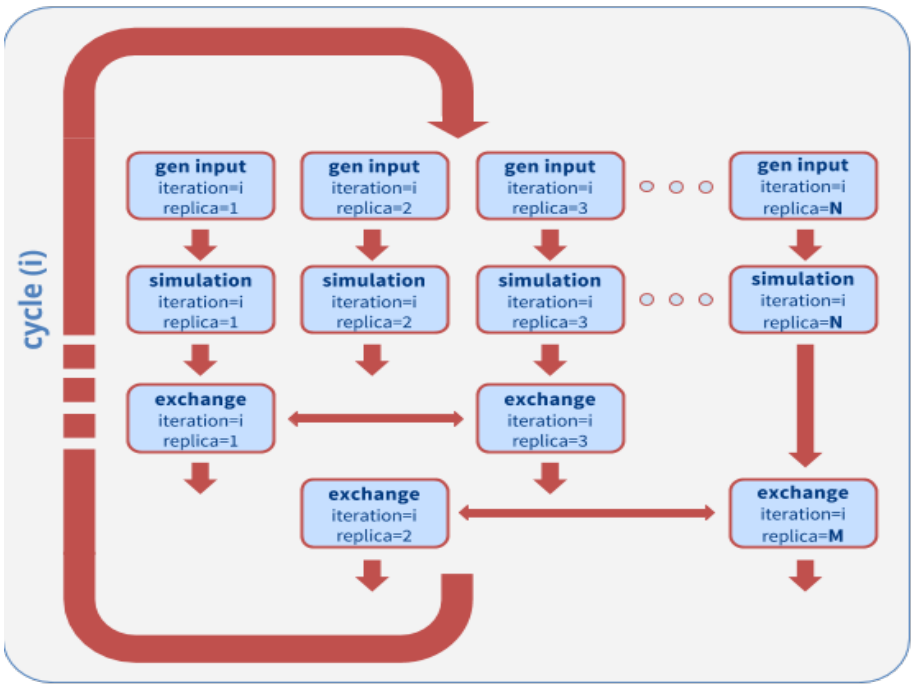
[23] depicts the execution of simulation and exchange phase with various degrees of concurrency depending on the number of iterations.

3.3.4 Simulation Analysis Loop

The Simulation Analysis Loop pattern is divided into two phases of simulation instances and analysis instances. There are also pre_loop and post_loop stages which are outside this iterative sequence. In the MD applications, the Simulation Analysis Loop pattern is executed with multiple iterations of simulation tool and analysis tool until the convergence criteria are reached. Figure 3.5 depicts N simulation instances and M analysis instances in each loop.

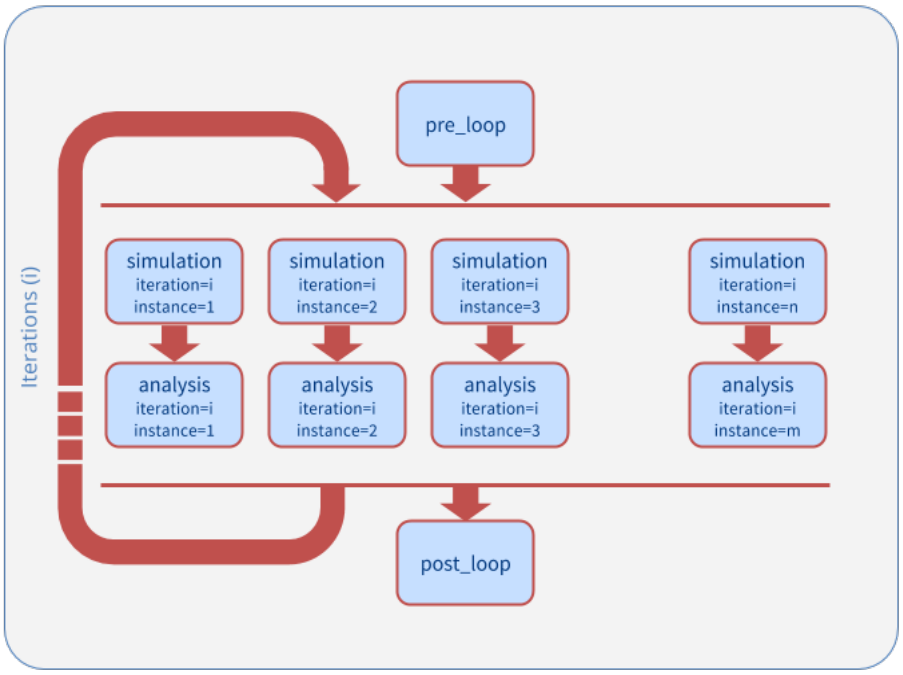
3.4 RADICAL RepEx Framework

RepEx is a framework for replica exchange molecular dynamics simulations over multiple dimensions. Replica exchange simulation deals with the exchange of thermodynamic information such as temperature, salt concentration or umbrella during molecule interactions, hence supporting 3-dimensional REMD simulations with an arbitrary ordering of the available exchange types [5], [24]. There are many REMD simulation tools that handles synchronous replica exchanges. In synchronous replica exchange, all of the replicas must finish the simulation phase before moving to the next stage, i.e. transition phase [5]. RepEx framework not only supports synchronous exchanges, but, it also manages the replicas that do not have global synchronization between the two stages, namely, simulation and exchange phase as shown in figure 3.6. This framework also handles resource allocation for the



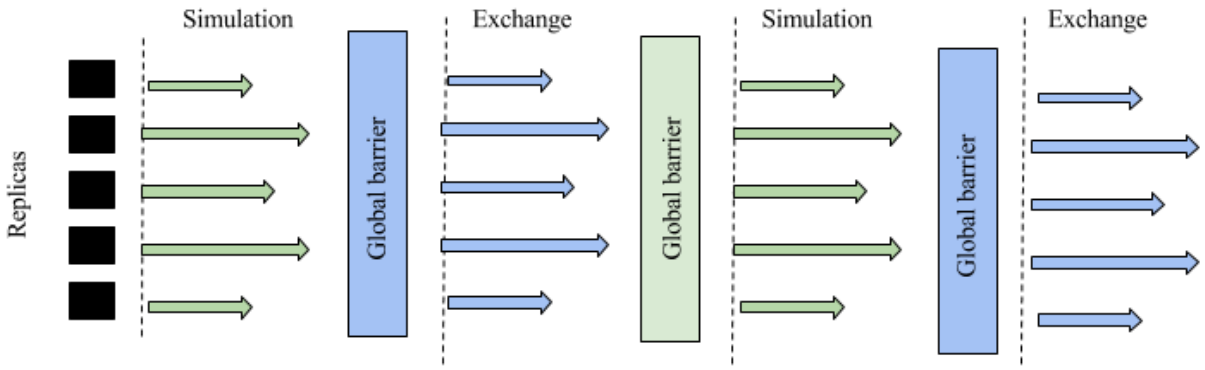
Credit: EnsembleMD toolkit architecture document [23]

Figure 3.4: Replica Exchange Pattern

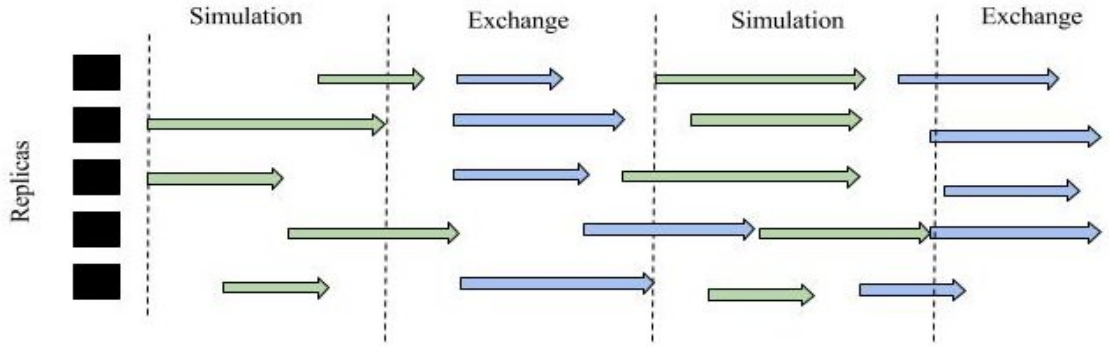


Credit: EnsembleMD toolkit architecture document [23]

Figure 3.5: Simulation Analysis Loop Pattern



(a) Synchronous REMD



(b) Asynchronous REMD

Figure 3.6: Schematic representation of REMD simulations [5]

HPC clusters using underlying RADICAL Pilot layer.

The main objective for the development of RepEx is to solve the concerns of the scientific community to implement REMD algorithms with a large number of exchanged parameters simultaneously providing a scalable platform with concealed simulation details.

Chapter 4
Software Testing Framework

Software testing is the primary way to improve software reliability. Software faults and errors could even cause huge financial damage to users, institutions or corporations. Automatic software testing reduces human efforts by testing the functionality and generating the output reports. This thesis mainly focuses on the development of a testing framework for the projects under RADICAL Cybertools Group such as EnsembleMD toolkit and RepEx framework. The earlier chapters focused on the EnsembleMD toolkit, its kernels, its patterns and underlying RADICAL-Pilot framework and concentrated on the importance and requirement of RepEx framework to enhance the domain of REMD simulations. In this chapter, we will discuss the various types of software testing and the importance of each type of testing in the field of software engineering.

4.1 Methods of Testing

Edsger W Dijkstra (1930-2002) says,"Testing can prove the presence of errors, but not their absence." In a broader view, testing methods can be divided into two subsections, namely: Static Test and Dynamic Test. These testing methods are also depicted in figure 4.1 for reference.

4.1.1 Static Test

In software development and testing, Static testing is a technique in which software is tested without executing the code. It gives comprehensive diagnostics for the code. This type of testing mainly has two components [35]:

- **Code Review:** It is typically used to find and eliminate the errors in the requirements, code, test cases or associated documents. This includes peer reviews.
- **Static Analysis:** The code written is checked for the proper structure, formatting, syntax correctness and code complexity. It can be tested manually or using some set of tools.

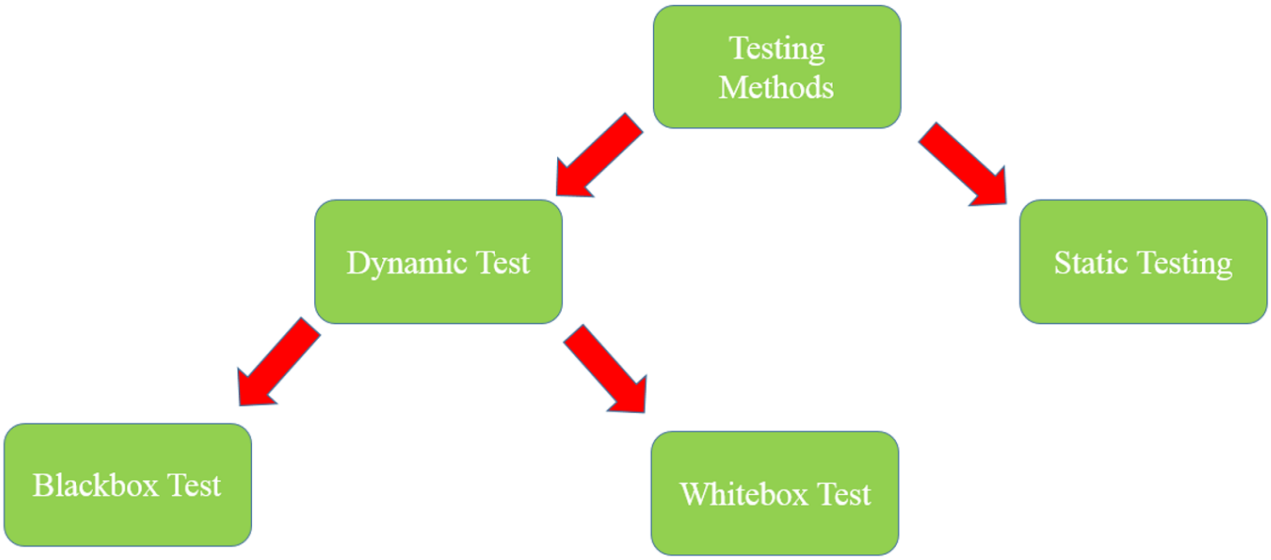


Figure 4.1: Methods of testing

4.2 Dynamic Test

This method is used to test the dynamic behavior of the code. It refers to the physical response of the system to various inputs. Unlike the Static test method, Dynamic tests require actual compilation and execution of the code. The actual output for the system for a given input is verified against the expected output. A dynamic test monitors system memory, functional behavior, response time, and overall performance of the system. The Dynamic test can be further divided into Blackbox test and Whitebox test.

4.2.1 Blackbox Testing

Software testing is required to test each module in the code so that maintenance cost can be reduced. Blackbox testing comes into picture when the source code is not available. Blackbox testing completely focuses on the output generated in response to the given input rather than the internal dynamics of the software [21]. This focuses on the functionality of the system rather than its implementation and deployment. Figure 4.2 shows the block diagram for blackbox testing where the implementation of the system under test is unknown. The only known parameters are the input and the expected output according to the system design document.

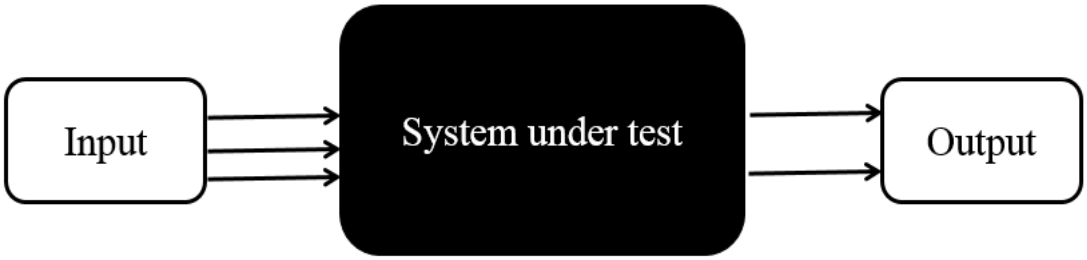


Figure 4.2: Block diagram of Blackbox Testing

4.2.2 Whitebox Testing

Whitebox testing, in contrast to blackbox testing, includes the knowledge of internal code implementation and code flow. In these types of test, all the individual paths, loops in the code structure and all the functions and methods are tested for their logical correctness. Whitebox testing is an important part of the SDLC of any developing software. A test engineer is required to have a full knowledge of the source code. These tests might be useful in detecting hidden errors, check dead code or other code related bugs [22].

4.3 Python Testing Tools

This section focuses on the study of different Python testing tools and selection of the most suitable tool for the testing framework. EnsembleMD toolkit is a Python-based framework and hence, Pytest is the most suitable testing tool for the same. The other tools for testing Python framework are Python Unittest/PyUnit, Doctest, Nose etc which are discussed briefly below.

4.3.1 Python Unittest/ PyUnit

Python's Unittest framework, developed by Kent Beck and Erich Gamma is based on the XUnit framework. PyUnit supports modularity and is flexible as tests can be organized into test suites with fixtures (setup/teardown). PyUnit supports test fixtures, test cases and a test runner to enable automated testing. The example of Unittest is below:

```
import unittest
class TestStringMethods(unittest.TestCase):
  def test_upper(self):
      self.assertEqual('foo'.upper(), 'FOO')
if __name__ == '__main__':
```

```
    unittest.main()
```

Output:

```
Ran 3 tests in 0.000s
OK
```

4.3.2 Doctest

Doctest is a simple testing framework that executes a shell script in docstring format in a small function at the bottom of the test file. Doctest enables the test by running examples included in the documentation and verifying the expected results. The test module searches for pieces of text that look like interactive Python sessions and then executes those sessions to verify that they work exactly as shown in the text. The example of doctest is below:

```
def mul_function(a, b):
>>>mul_function(2,3)
6
return a*b
```

Output:

```
Trying:
    mul_function(2, 3)
Expecting:
    6
ok
1 tests in 1 items.
1 passed and 0 failed.
Test passed.
```

4.3.3 Nose

Nose is an extension of Python Unittest to enhance testing. It has several built-in modules which help to capture error, output, code coverage. Nose, although fully compatible with Python Unittest, has a slightly different approach to running tests. Nose lowers the barrier to writing tests and its syntax is less complicated. The example of Nose test is below:

```
from unnecessary_math import multiply
 def test_numbers_3_4():
    assert multiply(3,4) == 12
```

Output:

```
Ran 1 tests in 0.000s
OK
> nosetests -v test_um_nose.py
simple_example.test_um_nose.test_numbers_3_4 ... ok
Ran 2 tests in 0.000s
OK
```

4.3.4 Pytest

Pytest is easy and has straightforward assertion statements. The failure output description of Pytest is better than other test frameworks. It provides a better description whenever the test case fails. Pytest framework has its own runner method to execute the tests with name test_*.py.

```
def func(x):
    return x + 1
def test_answer():
    assert func(3) == 5
```

Output:

```
======= test session starts ========
platform linux -- Python 3.4.3, pytest-2.8.7, py-1.4.31, pluggy-0.3.1
rootdir: /home/suvigya/radical.ensemblemd-master, inifile:
collected 1 items
test_sample.py F
======= FAILURES ========
_______ test_answer ________
    def test_answer():
>       assert func(3) == 5
E       assert 4 == 5
E        +  where 4 = func(3)
```

Automatic Test Execution	The primary requirement of the test framework is to execute the test automatically along with error reporting, test analysis and test report generation.
Convenience	Framework must be easy and convenient to use by the testers/ developers and must be easy to edit and add more tests.
Maintainability	Framework should be easy to maintain and update the test results as soon as any changes have been made in the source code or any changes have been pushed to the repository.

Table 4.1: Basic testing infrastructure requirements

```
test_sample.py:5: AssertionError
======== 1 failed in 0.12 seconds ========
```

The above results and the output of Pytest are more descriptive and hence, serves as the backbone for our testing framework over the other available test tools. Pytest not only provides better output logging, but also has simpler syntax, is easy to implement and is easy to integrate with continuous integration tools such as Jenkins or code coverage tools.

4.4 EnsembleMD and Repex Test Automation Framework Requirements

The previous sections discuss the different types of testing methods and tools available and superiority of Pytest over other testing tools. This section aims at the basic test structure and requirements of our test infrastructure.

4.4.1 High Level Requirements

The basic requirement of any test framework, especially EnsembleMD and RepEx framework, is described in the table 4.1.

4.4.2 Test Framework Capabilities

The flows chart in figure 4.3 depicts the capabilities of a test execution framework.

- **Starting or Stopping tests**

  As EnsembleMD toolkit and RepEx are evolving open source projects, where functionalities, APIs and source code is always changing and modified, it is important for the test infrastructure to start testing the updated source code with any newly pushed changes automatically. This

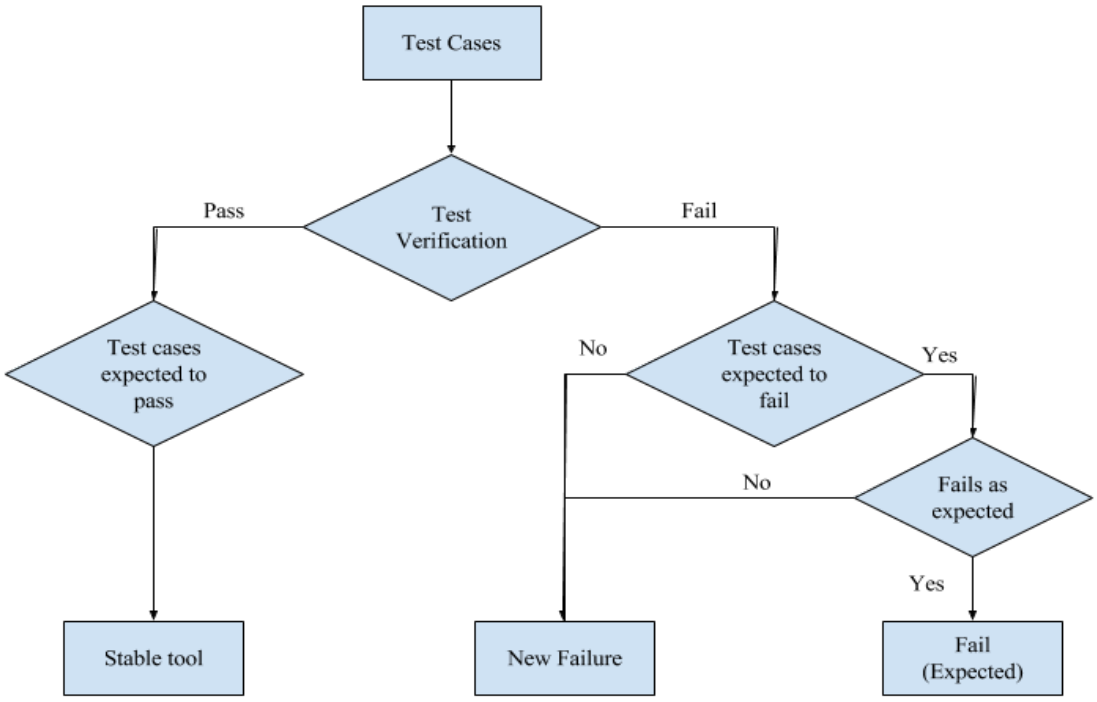


Figure 4.3: Test Execution Flow

ensures that the functionality of the overall system is intact and flawless. The framework should also start executing these tests at some frequent intervals to ensure that even a software upgrade on the remote HPC clusters are properly captured and source code of scientific applications is modified accordingly to make it compatible with the upgrades.

- **Test Report Generation**

  Test reports generated after each automated testing is very crucial. These test reports are not only important for test engineers, but also significant for the developers. Test reports elucidate developers about the failing modules. These reports provide steps or inputs to reproduce the error which is beneficial at the later stage to re-test the bug-fix provided by the developers.

- **Verifying Test Results**

  Verifying the test results is an integral part of test execution. Tests can be verified by comparing the actual output with the predefined expected output.

- **Handling Expected Failures**

  The essential part of any test execution is to verify and handle the failures. The analysis of the test failures is important to ascertain that the known to fail test cases have failed similarly as

expected or new defects have appeared. A test framework is expected to distinguish between the expected test failures and the new test failures on the basis of the expected output for a test failure.

The complete design of testing framework and the error detection is divided into 3 levels:

- **Development level testing:** This is the basic API level testing of the EnsembleMD toolkit and RepEx framework.
- **Deployment level testing:** This includes testing for the errors that occur during loading the environment, modules or the errors that arise during the transfer of scientific tool dependent input files on to remote machines.
- **Run-time testing:** This level of testing framework deals with the execution failure of scientific tools due to various reasons which are discussed in further chapters.

In our testing framework, Development level testing includes unit testing of all the independent APIs of EnsembleMD toolkit and RepEx framework which is discussed in the next chapter. We have designed Simple Application Testing Lite (SATLite), an independent framework for testing deployment and run-time level errors and faults. SATLite detects the errors using console logs of the supercomputer.

4.5 Types of Error

Table 4.2 focuses of the types of errors with is detected by this testing framework.

4.6 Limitations

The current version of this testing framework has been developed with a focus on MD applications. As discussed earlier, development level testing covers the unit testing and end-to-end testing, it consolidates RADICAL EnsembleMD and RepEx. Since RADICAL tools have a high dependency of external MD engines such as Amber, CoCo, Gromacs, etc. for simulation and analysis, it becomes difficult to design multi-path test framework to cover all the possible test execution paths.

SATLite tool can be generalized and scaled for the integration with applications other than MD applications. Miscellaneous applications such as simple mathematical software or hello world programmes can be used with the SATLite to detect the errors that might occur at the supercomputer during their execution.

Types of error	**Source of error**	**Remarks**
Source code bugs	RADICAL EnsembleMD and RepEx development code	These errors can produce unexpected results.
Improper or obsolete environment	Occurs on HPC cluster	Environment specific to MD engines are important for execution. Improper/ obsolete environment can cause the execution failure.
Improper input files	Can occur at local machine where the input files are erroneous. Can also occur at supercomputer due to improper transfer of files or transfer failure.	These files are important for execution. Errors due to wrong file can cause execution failure or erroneous results.
System failure	Occurs at HPC cluster	Errors generated while MD engine execution of HPC due to HPC system upgrades or hardware failures.
Segmentation Fault	Occurs in MD engine and HPC cluster.	These errors might occur when MD engines try to access illegal memory addresses.
Improper MD engine execution	Occurs at HPC cluster.	These errors occur due to job submission failure on HPC, job execution timed out or if job completed in unexpected range of time.

Table 4.2: Types of Error captured by Testing Framework

The current version of testing framework lacks the user study. The results of the bug capture during the development phase reports the error captured during EnsembleMD's and RepEx's execution on Stampede. The extensive testing on other HPC clusters can provide a broad list of errors specific to a particular HPC cluster. Also, SATLite has been tested only with the developed versions of MD engines and tested only with RADICAL Jenkins server. SATLite can be made more robust with an extensive user study. Its features can be further enhanced with a profound study of user behavior and requirements.

Chapter 5
Development-Level Testing

5.1 Introduction

The previous chapter briefly discussed the various testing tools and design features required for developing a test infrastructure for the EnsembleMD toolkit and RepEx. This chapter focuses mainly on the API level testing of all the pattern APIs, kernel APIs and execution handler APIs of EnsembleMD toolkit. The testing infrastructure is divided into Unit Testing, End to End Testing and Exception testing which is described in detail in this chapter.

5.2 Unit Testing

Unit tests are written and executed by the developers to ensure that the output of the code meets the design of the software. In the field of software programming, Unit Testing is a method to test the individual modules or units of the code to verify its proper functioning.

Pytest was chosen because of the following features:

- It collects all the test files automatically as it looks for file names starting with test_*.py.
- It has simple asserts and highly customizable debugging logs and output.

5.2.1 Unit Test for EnsembleMD Toolkit

All of the different APIs of all the patterns forms the building blocks of the EnsembleMD toolkit. Different APIs of a pattern can execute as an individual module with or without data dependency from previous stages. In general, Unit Testing for EnsembleMD toolkit pattern is divided into three modules as shown in figure 5.1, namely:

- **Basic API Test module:** It tests the basic APIs of the patterns viz import module test, the name of the pattern, check the variables etc.
- **Not Implemented Error test module:** The important feature of EnsembleMD toolkit is to generate the error and throw an exception when the pattern API or function is not defined

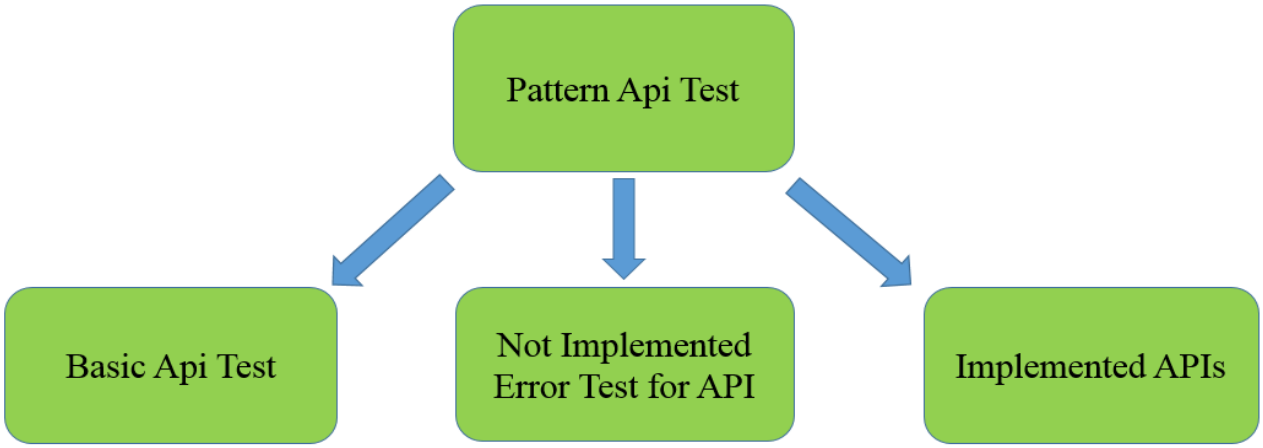


Figure 5.1: Unit Testing modules

or given any functionality. In this case, toolkit raises `NotImplementedError` error. In this module, we test the function without definition and the exceptions raised.

- **Implemented API module:** In this module, we define the APIs of the pattern and provide them functionality. These functions are given required inputs and are tested for the expected output. This tests all the APIs which generated `NotImplementedError` by defining them and executing them with specific input data or files.

Table 5.1 shows all the APIs of the patterns which were included in unit testing.

5.2.2 Unit test for RepEx toolkit

Unlike EnsembleMD toolkit, RepEx framework is a modifiable and scalable REMD simulation package that supports Amber and Nanoscale Molecular Dynamics (NAMD) as MD application kernels. The most important stage in any replica exchange simulation is the initialization of the replicas and the number of replicas in each dimensional group. Errors propagate to the next stage if the initialization of replicas is faulty and hence providing erroneous results. These errors in the final output might cause severe damages if the results are used in the development of drugs [1].

As discussed earlier, RepEx supports one-dimensional simulation with temperature exchange, umbrella sampling and salt concentration. These one-dimensional simulations can be combined to perform multidimensional exchange simulations. The test cases for the RepEx extensively focuses on the replica initialization part. Table 5.2 shows the important test cases scenarios of RepEx. These test cases are executed for all the dimensions for all the possible combinations; moreover, these test cases also checks for errors in synchronous and asynchronous modes of execution.

Pattern	**Basic API**	**Not Implemented API**	**Implemented API**
Pipeline	• import pipeline module • name • instances • steps	• step_n	• step_n
AllPairs	• import • name • permutations • set1_elements • set2_elements	• set1element_initialization • set2element_initialization • element_comparison	• set1element_initialization • set2element_initialization • element_comparison
Replica Exchange	• import • name • add_replica/ get_replica	• initialize_replica() • build_input_file • get_swap_matrix • perform_swap • prepare_replica _for_md • prepare_replica _for_exchange • exchange	• initialize_replica() • build_input_file • get_swap_matrix • perform_swap • prepare_replica _for_md • prepare_replica _for_exchange • exchange
Simulation Analysis Loop	• import • name • iterations • simulation _instances • analysis _instances • simulation _adaptivity	• pre_loop() • simulation_step() • analysis_step() • post_loop()	• pre_loop() • simulation_step() • analysis_step() • post_loop()

Table 5.1: Pattern APIs for Unit Testing in EnsembleMD toolkit

Test Cases	**Usage**	**If test fails**
test_initialize_replica_id	Tests the IDs of all the replicas that are initialized.	Wrong replica IDs would lead to improper exchange and tracking of replicas at the later stages.
test_total_group	Tests the total number of groups generated.	Incorrect group number would lead to improper exchanges.
test_group_d1	Tests for the proper number of replicas in D1 dimension.	Incorrect numbers would lead to error propagation to next stages and improper exchanges.
test_group_d2	Tests for the proper number of replicas in D2 dimension.	Incorrect numbers would lead to error propagation to next stages and improper exchanges.
test_group_d3	Tests for the proper number of replicas in D3 dimension.	Incorrect numbers would lead to error propagation to next stages and improper exchanges.
test_simulation	Tests for the proper exchange of parameters after each cycle.	Incorrect exchange of parameters would lead to erroneous output in the analysis stage.

Table 5.2: Test cases for Unit Testing in RepEx

5.3 End-to-End Testing

End-to-end testing tests the complete functionality of all the patterns starting from the selecting pattern, defining kernel and allocating the resource. Each pattern is tested with a specific input and compared with the expected output. These tests ensure the proper functioning and behavior satisfaction of the complete toolkit. The End-to-end testing on different supercomputers helps in establishing the reliability of the toolkit.

End-to-end testing includes testing all of the miscellaneous kernels along with the scientific tool kernels (Amber, CoCo, Gromacs and LSDMap). These tests are executed on both the localhost and Stampede supercomputer.

Test Case	**Exception Raised**	**Remarks**
test_TypeError	radical.ensemblemd.exceptions. TypeError	TypeError is thrown if a parameter of a wrong type is passed to a method or function.
test_FileError	radical.ensemblemd.exceptions. FileError	FileError is thrown if something goes wrong related to file operations, i.e., if a file does not exist or cannot be copied.
test_ArgumentError	radical.ensemblemd.exceptions. ArgumentError	This exception is thrown if a wrong set of arguments are passed to a kernel.
test_NoKernelPluginError	radical.ensemblemd.exceptions. NoKernelPluginError	This exception is thrown if no kernel plug-in could be found for a given kernel name.
test_NoKernelConfigur-ationError	radical.ensemblemd.exceptions. NoKernelConfigurationError	This exception is thrown if no kernel configuration could be found for the provided resource key.

Table 5.3: Test cases for raising exceptions

5.4 Exception Testing

The EnsembleMD toolkit and RepEx provides a well-detailed logging for the errors and exceptions. It generates very specific exceptions which help in debugging the failure at any step. We provide wrong or improper inputs to check if these exceptions are raised. Table 5.3 shows important exceptions provided by the two RADICAL toolkits.

Chapter 6
Deployment and Run-time Testing

Deployment testing is the next level of testing that captures the exceptions, faults and errors that might occur during the deployment of input files on HPC cluster or loading the scientific tool specific modules and environment onto the supercomputer. Run-time testing focuses on the exceptions that occur due to system failure or segmentation faults. In this thesis, we have carefully designed a framework that checks for the above-discussed levels of testing. Simple Application Testing Lite (SATLite) is primarily developed with an objective to test errors and exceptions which occur during the execution of scientific tools (Amber, Coco, Gromacs, LSDMap etc) on remote supercomputers.

According to [6], 1.53% of the total applications on Blue Waters supercomputer failed because of the system problems. Such system failures have a great impact on the computing resources and financial budgeting. The majority of testing tools that have been developed focuses on testing the failures due to system faults, both software and hardware. LogDiver, a tool primarily developed by Martino et al. [6] analyzes the system level faults. Failures in HPC clusters have become more prominent with the enhancement in the number of components. The exponential increase in the failures calls for immediate actions to minimize the effect of failed applications on the high computing resources. In this chapter, we focus on application side failure detection.

6.0.1 Basic Definitions

A few terms related to the development of testing frameworks are discussed below:

- **Modules:** Basic environment for the default compilers, tools and libraries. Users requiring 3rd party libraries or tools can tailor their environment with the applications and tools they need. Module and environment can be used interchangeably.
- **Files:** User's input files specific to the scientific tool
- **Supercomputer:** These are the HPC resources that are used for the execution of applications. HPC cluster, remote machines and supercomputers can be used interchangeably.

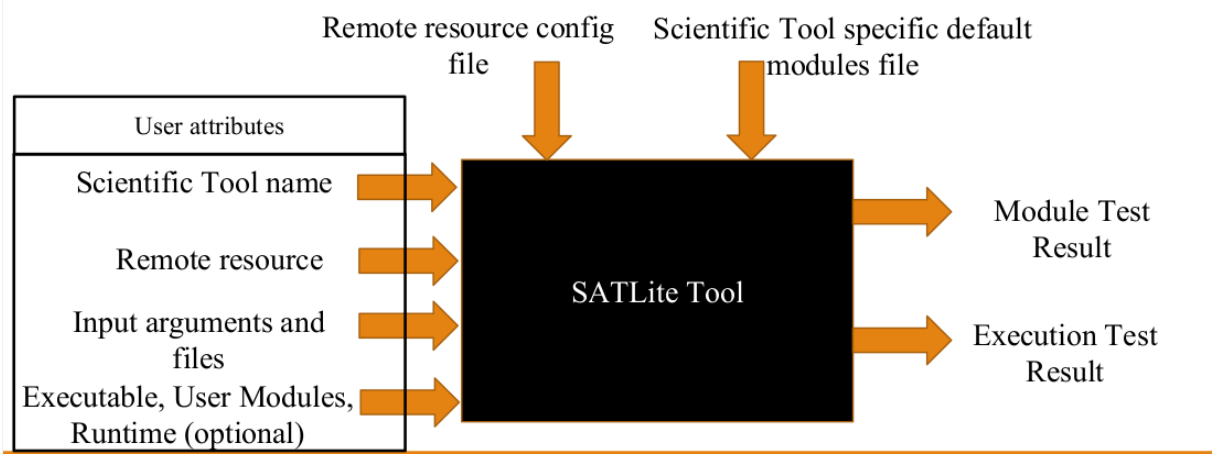


Figure 6.1: SATLite System Design

- **Scientific tools:** These are the MD simulation and analysis tools such as Amber, CoCo, Gromacs and LSDMap.

SATLite tool can help the developers of the scientific community, especially the MD community to investigate the errors and issues that may be generated due to their software bugs or the remote system changes and upgrade. This enables them to test the changes which have been made in their tools before releasing it for their users. The errors and exceptions might occur due to the following occurrences:

- Improper or obsolete module loading.
- Improper input arguments or input files.
- System failure or segmentation fault.
- Failure as the execution did not complete in expected range of time.

6.1 SATLite System Design

Figure 6.1 shows the block diagram of the system. SATLite tool performs the test in two steps, i.e. Module Test and Execution Test. In figure 6.1, user attributes field depicts the APIs exposed to the users. These APIs are explained in the later sections. Resource configuration file and scientific tool specific defaults modules file serves as the input to this testing tool.

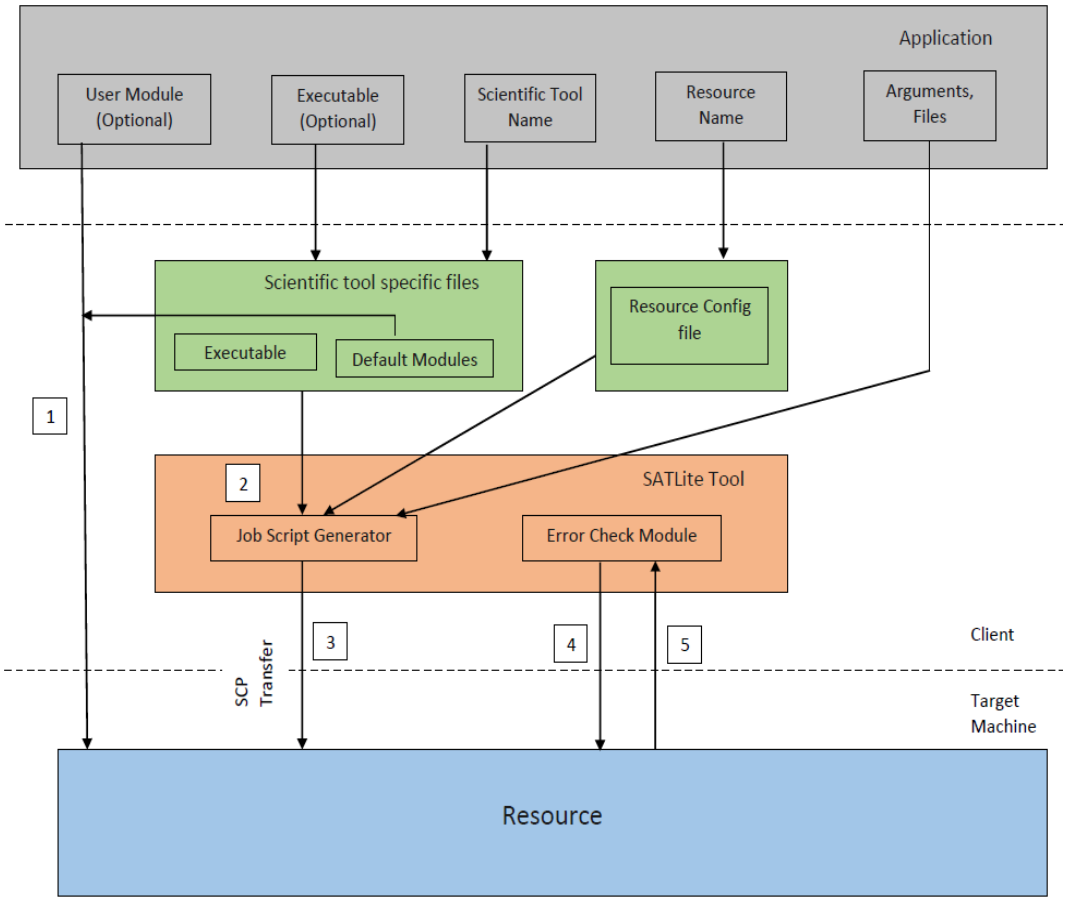


Figure 6.2: SATLite tool architecture

6.2 System Architecture

As a part of SATLite design and development, the primary focus is to report the exceptions and errors occurred due to the inadmissible loading of the environment or improper input files on the supercomputer. The continuous development of the scientific tools and changes in their source code raised a requirement to develop a tool that can report any errors relating to its execution on the remote supercomputers.

SATLite tool provides a set of explicit APIs to the users to test their own scientific tool or application. It has been currently tested for Amber, CoCo, Gromacs and LSDMap. The environment loading, file transfer, job scheduler script generation and its execution is hidden from the users, hence, they can solely focus on the development of scientific tools rather than concentrating on debugging the errors and exceptions.

6.2.1 Control Flow

The control flow for two stages of the SATLite as shown by specific numbers in figure 6.2 are discussed below.

Module Test

{1} Load user provided or defaults modules on the supercomputer and wait for the console logs. If the user does not explicitly provide any input modules, then the default modules from the scientific tool specific file are used. These console logs are examined to check for the errors during the environment loading stage. If any error event occurs at this stage, the logs are written to the module_error log file explaining the possible reason for failure.

Execution Test

{2} Generate job scheduler script using scientific tool executable, modules for a specific remote machine using remote machine configuration file.
{3} All of the input files along with the scheduler script is transferred to the remote machine using Secure Copy Protocol (SCP). The errors and exceptions are detected, if any, during the file transfer stage. If all the files are transferred successfully, the job is submitted to the computing resource queue where the tool waits for execution to complete.
{4} Output files and error files are generated and these log files are examined to detect any failure during execution.
{5} At the last stage, errors are reported back to the users. Also, all the output files and error files are transferred back to the local machine.

6.3 System Log Collection and Processing

We begin by examining the details of the cluster, event methodology and then it's processing.

6.3.1 About the Cluster: Stampede

We have currently tested SATLite on the Stampede supercomputer from TACC. Stampede is one of the most powerful supercomputers which went into production in 2013. In 2012, a pre-production configuration of Stampede used 1875 nodes which were then expanded to 6400 nodes with a total memory of 205 TB. The project was built in partnership with Intel, Mellnox and Dell. Table 6.1 shows the technical details of Stampede.

Resource	Specification
# of Nodes	6400
Processors	Xeon E5-2680 8-core processors
Co-processor	Xeon Phi coprocessor
Memory	32 GB RAM, 205 TB total memory
GPU	Nvidia Kepler K20 GPUs
Operations	9.6 quadrillion floating point operations per second

Table 6.1: Stampede system specifications

6.3.2 Event Logs and Processing

Supercomputers such as Stampede logs all of the events that occur during the complete execution of the application. System logs serve as the repository of the event data. Console logs provide the real-time job status. We have utilized these console logs to detect the deployment time and run-time errors. In the deployment stage, it is highly likely that the modules required to run a scientific tool and workflow are erroneous or have become obsolete. The events generated on the console logs are analyzed to provide the explanation of the error.

In the run-time stage, we have used console logs to extract job id, job status, execution time etc. When a batch job exits [6], Stampede generates an exit code which shows the completion status. A successful and exception-free execution returns ExitCode 0 as a return code, otherwise an integer greater than 0 depicting the different type of errors and exceptions. It is also possible that a job can finish successfully even if the application has terminated abnormally. To address this case, we have used the actual execution time to complete and checked if it lies in the expected range of completion time.

6.4 SATLite Tool Components

The components exposed to the users are discussed below. These components are the parameters that are required to be set using `set_attribute()`.

6.4.1 Scientific Tool Name

This is the field where the user has to provide the scientific tool name (currently supported scientific tool name are Amber, CoCo, Gromacs and LSDMap) that has to be tested. For example,

```
name = amber
```

6.4.2 Resource Name

The input to this field is the name of the supercomputer or any target machine where the execution of the scientific tool has to be checked. This currently supports SLURM job scheduler. For example,

```
resource = xsede.stampede
```

6.4.3 Arguments

The list of input files specific to the scientific tools along with the arguments is provided in a specific format as shown in the example below.

```
arguments = ['argument1=input_file1','argument2=input_file2]
```

6.4.4 Exe

This is an optional field where the users can provide their executable which then overrides the default executable.

6.4.5 User Modules

This is an optional field where the user can explicitly provide the required environments. The inbuilt modules specific to scientific tools (Amber, CoCO, Gromacs and LSDMap) are used if no user modules are provided.

6.4.6 Run-time

Users can provide an estimated range for run-time to check for additional execution failures if no exit code or error is found. The actual run time of the execution should lie in the runtime range provided by the user. It is provided in the following format:

```
runtime = [''min_time(hh:mm:ss)","max_time(hh:mm:ss)"]
```

Function Name	Arguments	Description
set_attribute	• name, • resource, • arguments, • exe (optional), • modules (optional), • runtime (optional)	Sets all the required attributes for execution
run	void	Executes test

Table 6.2: Exposed SATLite tool APIs

6.5 Execution

There are two ways for the users to execute the SATLite, namely:

- Command Line Tool
- Use the exposed APIs in the code.

6.5.1 Command Line Tool

To run SATLite using command line tool, users are required to provide the scientific tool name, target remote machine and arguments file or a file with the list of input files that are required for the execution of the scientific tool. Users can also provide optional executable name and module file explicitly. They can also provide optional execution runtime range. It is recommended to provide a runtime range to enhance the failure reporting. The resulting invocation of SATLite should be:

```
python satlite_exe.py --name <scientific_tool_name> --resource
<target_resource_name> --arguments <argument_file> --exe <Optional
_executable> --modules <optional_module_file> --runtime <Optional
_runtime_range>
```

Where,

```
scientific_tool_name = Scientific Tools (Amber, CoCo, Gromacs, LSDMap)
target_resource_name = Remote Supercomputer Name (Currently tested on
```

```
                        Stampede)
argument_file         = File of list of input files with arguments
Optional_executable   = Executable
optional_module_file  = File with list of modules
Optional_runtime_range= Runtime range in format [min_time, max_time] in
                        hh:mm:ss
```

6.5.2 Use the Exposed APIs in the Code

This section provides a guide for using the APIs exposed to the users. The below-mentioned example executes Amber on Stampede.

```
"""
Sample Code
"""
from satlite import SATLite

if __name__ == "__main__":
    test = SATLite()
    test.set_attribute(name = 'amber',
                       resource = 'xsede.stampede',
                       # amber
                       arguments = ['-O',
                               '-i=/home/suvigya/inp/min.in',
                               '-p=/home/suvigya/inp/penta.top',
                               '-c=/home/suvigya/inp/penta.crd',
                               '-inf=/home/suvigya/inp/min.inf',
                               '-r=/home/suvigya/inp/md.crd',
                               '-ref=/home/suvigya/inp/min.crd'],
                      #Executable optional
                      exe = sander
                      #amber modules optional
                      modules = ["module load TACC",
                             "module load intel/13.0.2.146",
                             "module load python/2.7.9",
```

```
                    "module load netcdf/4.3.2",
                    "module load hdf5/1.8.13"]
                runtime = ["0:0:1","0:0:15"]
            )
    test.run()
```

6.6 Features of SATLite Tool

This section focuses on various design features of the SATLite tool that make it an abstraction level scalable solution for detecting deployment and run-time faults.

- It is highly scalable as it can test a large number of miscellaneous kernels and executables in addition to the scientific tool kernels.
- This tool supports multiple independent executions, hence saving user's time in submitting different jobs separately.
- If scientific tools are being tested, users can explicitly provide an environment list to load on the remote machine. If the environment list is not provided by the user, the tool uses default modules from the scientific tool configuration file. This feature enables the user to override the obsolete environment and module list provided by the tool.
- SATLite also detects the error caused due to improper execution of the job leading it to complete execution successfully in an unexpected range of time. For instance, the execution of a job with 1000 input files takes 5 seconds to complete on a remote machine might return a successful execution, but if the absolute time to completion is more than the actual time depicts that execution is erroneous. Users can optionally provide an estimated range for the run-time to check for additional errors and exceptions.
- SATLite tool also checks for similar files that are required by multiple jobs before transferring them to the remote machine. This limits the number of file transfers to the remote machine, hence saving resources.
- The errors encountered are also written to the local machine in module_error log files for further investigation.

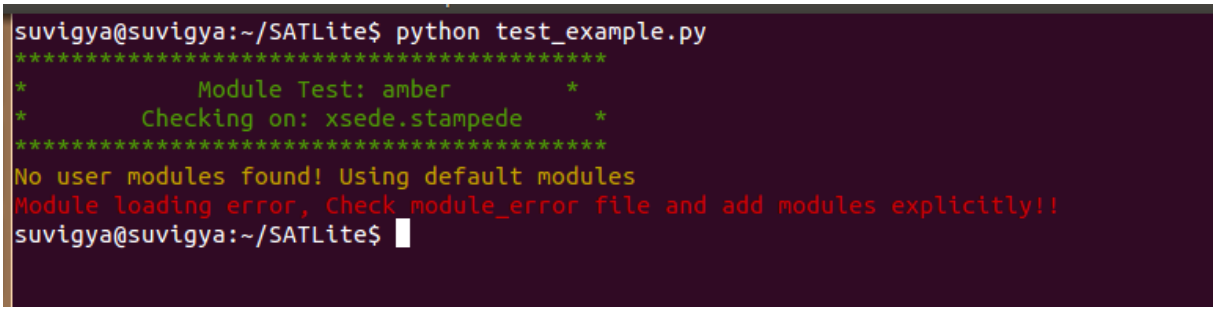


Figure 6.3: Failure due to improper module loading

In Figure 6.3 execution failed as the modules required for the execution of Amber on Stampede had errors.

6.7 Steps to Use SATLite

This section focuses on the steps for the users to exploit the features of SATLite to detect the errors and debug them.

STEP I: User runs SATLite with required MD engine name, remote resource name, required input files and arguments using command line or the exposed APIs.

STEP II: SATLite reports the error, if any, during the environment loading stage. If there are any errors, the execution terminates.

STEP III: If failure occurred during step II, user can use `module_error.log` file to debug the error.

STEP IV: If step II is successful, SATLite proceeds to execution stage. It transfers all the input files provided by the user to the HPC cluster. It reports error during the tranfer of files.

STEP V: SATLite submits the job to the batch queue and waits for execution. Users are reported the errors, if any occurred, during execution.

STEP VI: Errors discussed in Table 4.2 are reported by SATLite and can be used by users to debug the failures.

6.8 Expected Output

The main objective of SATLite is to detect and report the execution errors and exceptions, this section discusses the expected output in case of execution failure or success.

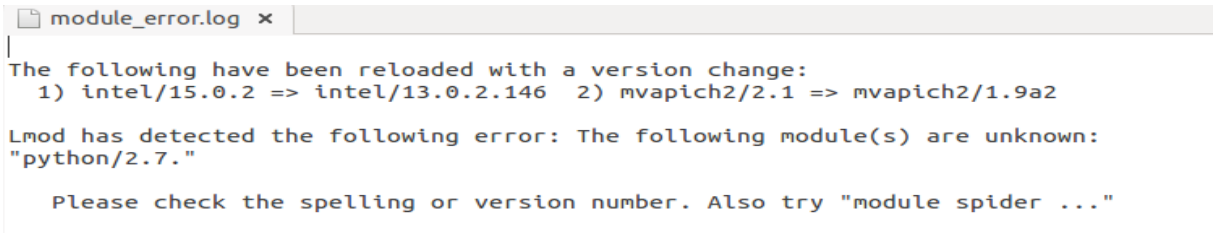


Figure 6.4: Example of module_error log file

Figure 6.4 shows an example of module_error log file which provides explanation of possible error.

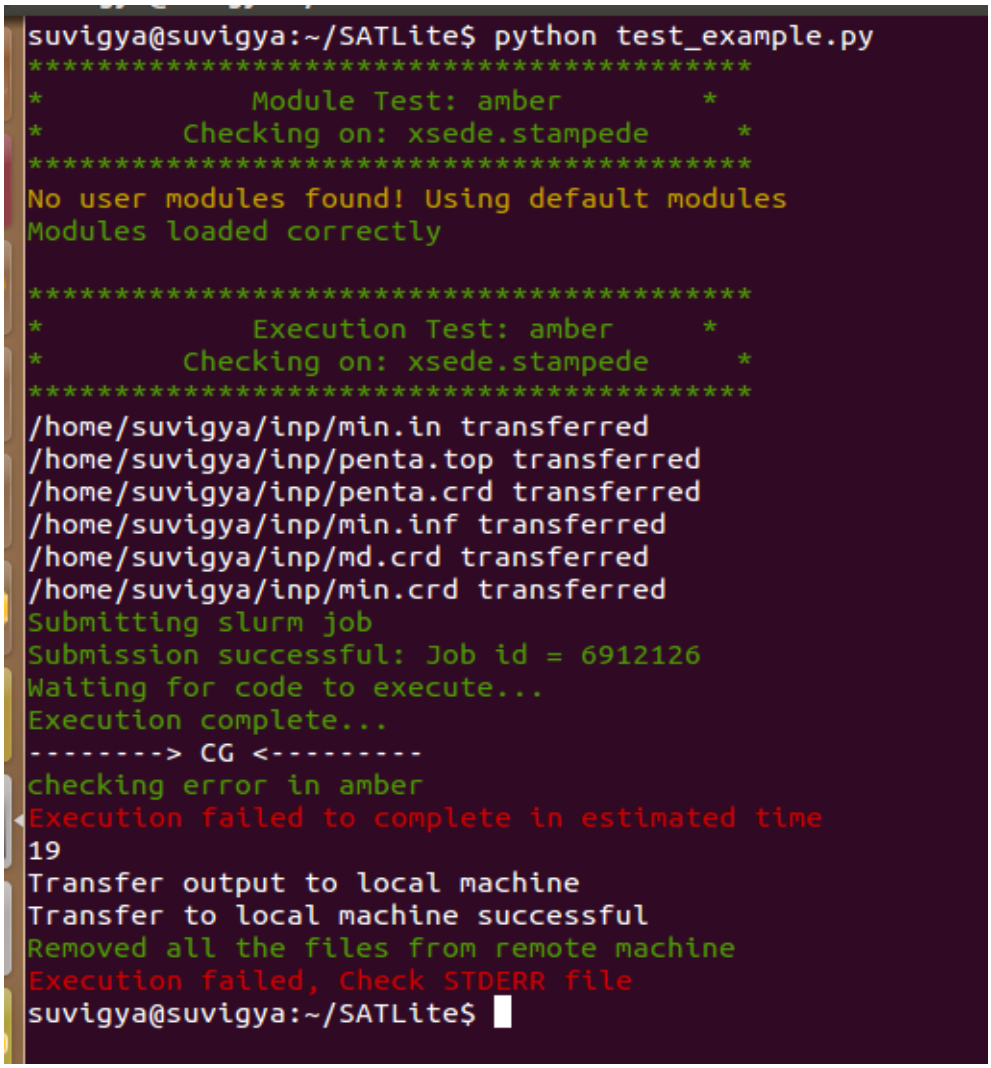


Figure 6.5: Execution failed to complete in the estimated time

In Figure 6.5, the tool reported an error as the execution failed to complete in the estimated range provided by the user.

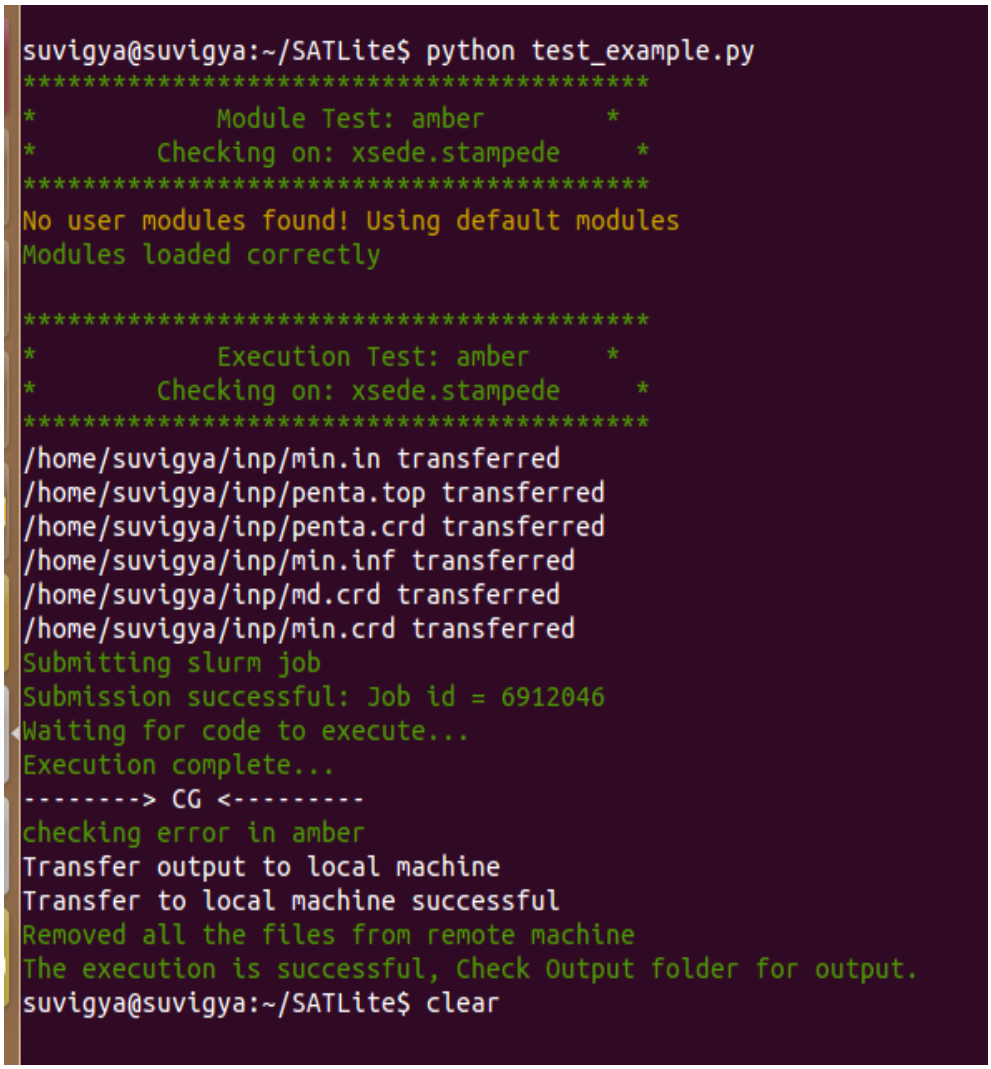


Figure 6.6: Successful Execution

In Figure 6.6, tools reports successful execution as no errors or exceptions were reported during the execution.

Chapter 7
Continuous Integration

Manual testing at times can be a laborious and time-consuming process. Sometimes it is not feasible and efficient to test the same modules every time if a small change has been made. This difficulty further increases with the increase in complexity of components in a software product. Even a single component change in such a complex and interdependent system can affect the behavior of other modules. This requires an urgency to implement an automated testing framework that can reduce manual testing work and simultaneously test all the critical components of the system. Continuous integration is a software engineering principle of rapid and automated development and testing. As discussed by Betz et al. [13], a continuous integration and central testing repository help the developers to identify a broken test case or failure with certain compilers automatically whenever a change is pushed.

Testing is an inevitable part of any project and it is required to be automated and integral to the build process so that developers do not have to manually test every aspect of their code.

7.1 About Continuous Integration

The complete source code is required to be pushed on to central repository. GIT is the most common tool used for version control by recent day developers. Github provides online free code repository. Since, the major work done by the scientific community, especially RADICAL Group, is open source, Github becomes an obvious choice for controlling and maintaining our code repository. In a continuous integration lifecycle, an automated system gets triggered when developers push their revised code on the repository. This system picks up the changes, pulls down the code and execute a few sets of commands to verify that the application still works as expected even after the code modification [14]. The most difficult part was to select the continuous integration server which would serve our purpose and execute our development stage unit cases for EnsembleMD and RepEx along with SATLite tool for testing deployment and run-time error reporting. The primary reasons for building an automated testing system are:

- **Time saving:** Developers can save a considerable amount of time testing their build by

automating the build and test phase.

- **Improved software qualities:** Any detected issues can be resolved immediately, hence keeping software in a state where it can be safely released at any time.
- **Faster development:** Development and release of any software is faster since manual integration issues are less likely to occur.

7.2 Principles of Continuous Integration

The software engineering practice of continuous integration was used to create a common build and test environment that integrates the developers' code into one test environment and hence, errors can be detected on a commit basis [13]. This section focuses on the main principles involved in the designing of continuous integration.

A. Maintain a Single Repository

One of the most important aspects of continuous integration is to maintain a single and central repository. This allows keeping track of multiple files and code changes. Maintaining a single repository can also prevent divergence in the code that could lead to difficult in resolving conflicts close to release.

The current EnsembleMD and RepEx development process maintain a common Git repository for the source code. This feature has been extended to maintain a separate repository for the testing framework of the former tools.

B. Automate the Build

As the project gets larger and bigger, it becomes important that developers do not spend time in typing commands to compile, build and test the source code. The automated test build software ensures the efficiency and also allows the easier support for many build options, such as building in a virtual environment, execution on multiple supercomputers, etc.

C. Make the Build Self-testing

All software needs testing to eliminate source code bugs. Testing is a significant part of the SDLC and validation needs to be automated and integral to the build process. The continuous integration is expected to build the code changes pushed to a central repository automatically and execute the testing suite to ensure that it behaves as expected by the developers.

D. Frequent Commits

The practices of continuous integration encourage developers to commit their code changes as often as possible. This is beneficial to avoid merge conflicts if two developers are unknowingly modifying the same segment of the code. It is easier for the developers to merge, move, add or remove the code changes if the commits are more modular. Committing the code marks a point in the history of the code base where developers can switch back and use the changes made.

E. Testing in a Clone of Production Environment

It is highly likely that the production environment used by the end user is different from the development or the test environment. The testing environment should be close to the production environment. This principle aids in finding errors that may not be present on the developers' machine.

F. Build and Test Result Availability

According to this principle, it is important to have a current development and staging build available at all times. Along with the build, the test result availability provides a visibility on the results to the developers.

7.3 Selecting Continuous Integration Server

The previous section discussed the principles and guidelines required to design a complete automated continuous integration server. There are a lot of existing and open source CI servers, namely, Jenkins [31], GitLab [32], Hudson, Cruise Control, TeamCity [33], Travis, Cider [15], etc. Selecting the best and optimal CI server is the most arduous task. The most suitable continuous integration server should have certain features as discussed in table 7.1. We have conducted a detailed study of the various available CI servers based on various features. Jenkins is Java based and is the most popular CI server which is compatible with most of the operating systems and many languages. Moreover, it has multiple plug-ins to configure the required system-of-interest. Travis is also a commonly used CI server where each project runs in an individual virtual machine [23]. Testing open source projects in Travis is free of cost, but there is a charge for private repositories. TeamCity, developed by JetBrains, is an excellent paid CI server; whereas, Jenkins is a free open source server. TeamCity is extensively used in large organizations. GitLab is a more recent application which integrates source code management and a CI server, but it does not support as many plugins and languages as is

Sr No.	Feature	Remarks
1.	Version control system integration	CI system should support the integration with all the version control systems.
2.	First-time setup	CI system is expected to guide through the first time steps to setup the project.
3.	User Interface	CI system at minimum is expected to provide an overview of all the builds and allows to examine each specific build for more detailed information.
4.	Build Environment	CI system should support a large number of programming languages and has extensive configuration properties.
5.	Feedback and reporting	CI systems should have mechanism to notify developers about the bugs or the issues.
6.	Post-build setups/ deployments	CI server should be able to deploy artifact to staging server, send emails, update bug, generate reports etc.
7.	Ease of extensibility	CI systems should be extensible and should provide large number of plug-ins.

Table 7.1: Features of CI system

supported by Jenkins [13], [14], [17]. Table 7.2 summarizes and compares the different CI servers that were considered in the study.

7.4 Reasons to Select Jenkins

The extensive research of different CI server has led us to choose Jenkins. Jenkins is very well established and extensively utilized CI server due to the following reasons:

- **Available Plugins:** Jenkins currently supports 392 plug-ins. It is a hub for the development of a large number of projects and applications due to its powerful and diverse functionality.
- **Cloud-enabled:** Cloudbees provides unlimited cloud space to the Jenkins users to build and test their code.
- **Large number of developer:** Jenkins is maintained by a large number of developers who were initially members of the Hudson CI server. Since Jenkins has a team of well-experienced developers, the software releases and upgrades are usually stable.

Feature	**Jenkins**	**Travis**	**TeamCity**	**GitLab CI**
Source availability model	Free and Open Source	Free for open source project	Proprietary/ Closed source	Free and Open source
Customizable and Scalable	Highly customizable. Large plugin ecosystem	Supports dozens of languages.	Supports large number of languages and APIs for the extension.	Highly scalable. Tests can run on parallelly.
Operating System support	Supports Windows, Mac OS, Unix-like OS	OSX and Ubuntu. Windows not supported. Python is not supported on OSX	Supported on Windows, Mac OS, Linux	Supported on Ubuntu, Debian, CentOS. Not supported on OSX, Windows, Fedora.
Integration	Can be integrated with all the source code management software.	Supports integration only with GitHub.	Can be integrated with all the source code management software.	Officially integrates only with GitLab.
Tutorial and Documentation	Good tutorials available. Poor official documentation.	Extensive and helpful documentation available.	Well documented.	Well documented.
Cost	Free	Not free for private repos	Expensive	Free
Capability	Easy installation, easy configuration, distributed builds, and extensive plugins.	Easy setup, multiple test environments for different runtime versions, helpful community.	Easy installation, great user interface.	Quick setup for the projects hosted on GitLab

Table 7.2: Comparative study of CI servers

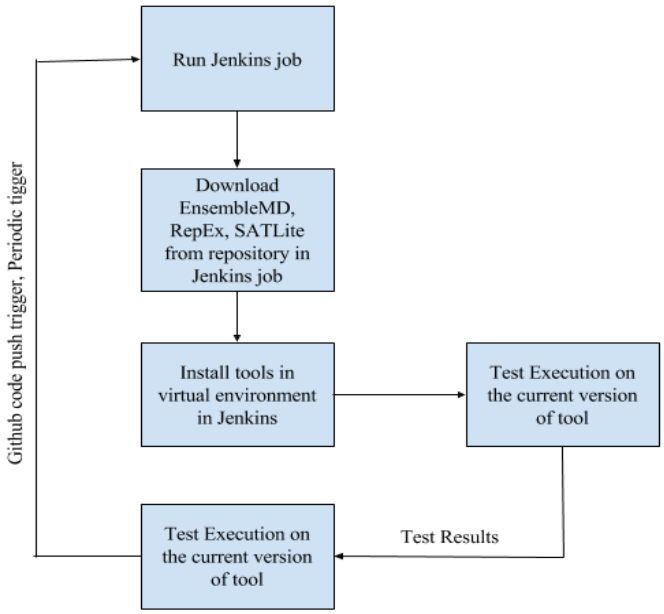


Figure 7.1: Test Process using Jenkins

7.5 Jenkins Integration

Jenkins is the obvious choice for automated test bench integration of our development, deployment and run-time testing of EnsembleMD, RepEx and SATLite tool. Figure 7.1 shows the stages in our Jenkins test process. The following are the generalized steps in integrating our testing with Jenkins:

- Jenkins job gets triggered whenever changes are pushed into the Github repository or builds periodically even if the code base in not modified. This periodic build ensures that unmodified code builds and executes successfully on the remote machines.
- Jenkins pulls the code from the tool repository and installs the tools in the virtual environment.
- It then clones the test cases and executes unit test using Pytest.
- Post-build generates a detailed test report showing the failure points, code coverage graphs, general trend in execution and violations in the Python code formatting as shown in figures 7.2,7.3, 7.4. 7.5, 7.6, 7.7 and 7.8.

```
+ py.test --cov-report term-missing --cov-report xml --cov=. ./patterns/test_allpairs_api.py ./patterns/test_pipeline_api.py
./patterns/test_replicaexchange_api.py ./patterns/test_simulationanalysisloop_loop_api.py -v --junitxml=./reports/pattern_api.xml
============================= test session starts ==============================
platform linux2 -- Python 2.7.6, pytest-2.9.1, py-1.4.31, pluggy-0.3.1 -- /var/lib/jenkins/shiningpanda/jobs/0237ac98/virtualenvs/d41d8cd9/bin/python2.7
cachedir: ../.cache
rootdir: /var/lib/jenkins/workspace/radical.ensemblemd.unittest/radical.ensemblemd, inifile:
plugins: cov-2.2.1
collecting ... collected 46 items

patterns/test_allpairs_api.py::TestBasicApi::test_import PASSED
patterns/test_allpairs_api.py::TestBasicApi::test_pattern_name PASSED
patterns/test_allpairs_api.py::TestBasicApi::test_pattern_permutatuions PASSED
patterns/test_allpairs_api.py::TestBasicApi::test_pattern_set_1_elements PASSED
patterns/test_allpairs_api.py::TestBasicApi::test_pattern_set_2_elements PASSED
patterns/test_allpairs_api.py::TestNotImplemented::test_pattern_set1_initialization PASSED
patterns/test_allpairs_api.py::TestNotImplemented::test_pattern_set2_initialization PASSED
patterns/test_allpairs_api.py::TestNotImplemented::test_element_comparision_not_implemented PASSED
patterns/test_allpairs_api.py::TestImplemented::test_set_1_initialization PASSED
patterns/test_allpairs_api.py::TestImplemented::test_set_2_initialization PASSED
patterns/test_allpairs_api.py::TestImplemented::test_element_comparision PASSED
patterns/test_pipeline_api.py::TestBasicApi::test_import PASSED
patterns/test_pipeline_api.py::TestBasicApi::test_pattern_name PASSED
patterns/test_pipeline_api.py::TestBasicApi::test_pattern_tasks PASSED
patterns/test_pipeline_api.py::TestBasicApi::test_pattern_number_stages PASSED
```

Figure 7.2: Each test case report

7.6 Post Build Actions

After Jenkins build has finished execution and build, it generates different reports in order to provide detailed logging of the build. This section focuses on the various reporting mechanisms used in continuous integration system.

A. Test Case Report

Test case report provides a detailed result of the tests included in the build. It shows each test case function name with the failure or success report as shown in figure 7.2.

B. Failure Report

Jenkins exploits the characteristics of Pytest that displays the possible reason for the failure. Figure 7.3 shows an example of the detailed failure report. This is beneficial to debug the code bugs and resolve them.

C. Code Coverage

Code coverage is a measure used to describe the extent of which the test code is tested by a test suite. A high code coverage shows that the program has been thoroughly tested and has lower chances of containing software bugs. Figure 7.4 and Figure 7.5 shows code coverage in tabular and graphical format respectively.

```
================================== FAILURES ===================================
_____________________ TestBasicApi.test_simulation_adaptivity _____________________

self = <test_simulationanalysisloop_loop_api.TestBasicApi object at 0x7f625c169790>

    def test_simulation_adaptivity(self):
        from radical.ensemblemd import SimulationAnalysisLoop

        pattern = SimulationAnalysisLoop(5,5,5)
>       assert pattern.simulation_adaptivity == False

patterns/test_simulationanalysisloop_loop_api.py:108:
_ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _ _

self = <radical.ensemblemd.patterns.simulation_analysis_loop.SimulationAnalysisLoop object at 0x7f625c169dd0>

    @property
    def simulation_adaptivity(self):
>       return self._simulation_adaptivity
E       AttributeError: 'SimulationAnalysisLoop' object has no attribute '_simulation_adaptivity'

../../../../shiningpanda/jobs/0237ac98/virtualenvs/d41d8cd9/local/lib/python2.7/site-packages/radical/ensemblemd/patterns/simulation_analysis_loop.py:125:
```

Figure 7.3: Example failure report

```
---------- coverage: platform linux2, python 2.7.6-final-0 ----------
Name                                                 Stmts   Miss  Cover   Missing
----------------------------------------------------------------------------------
__init__.py                                              1      1     0%   2
patterns/test_allpairs_api.py                           88      0   100%
patterns/test_pipeline_api.py                           28      4    86%   25, 28-31
patterns/test_replicaexchange_api.py                   175      0   100%
patterns/test_simulationanalysisloop_loop_api.py        82      1    99%   57
slow_test.py                                            19     19     0%   1-21
----------------------------------------------------------------------------------
TOTAL                                                  393     25    94%
Coverage XML written to file coverage.xml
```

Figure 7.4: Code Coverage: Tabular format

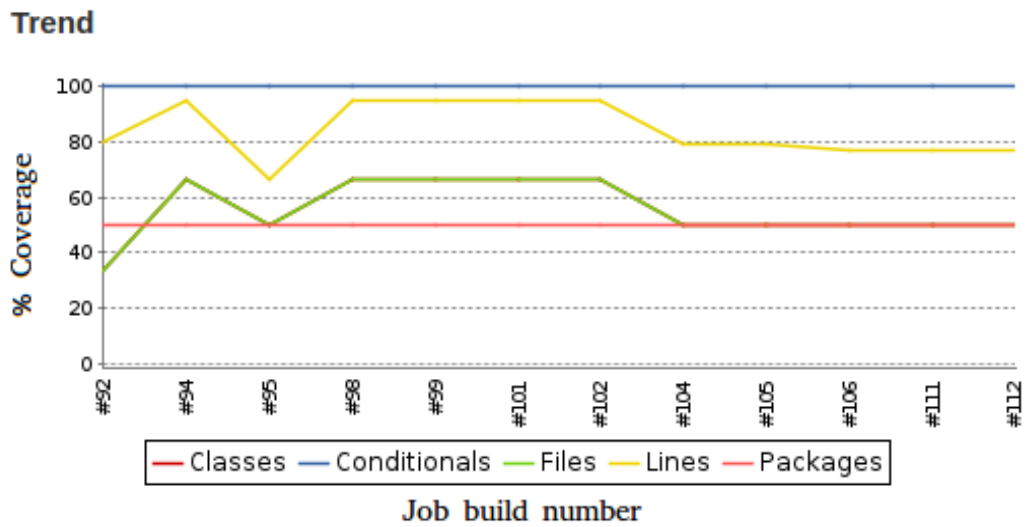


Figure 7.5: Code Coverage: Graphical format

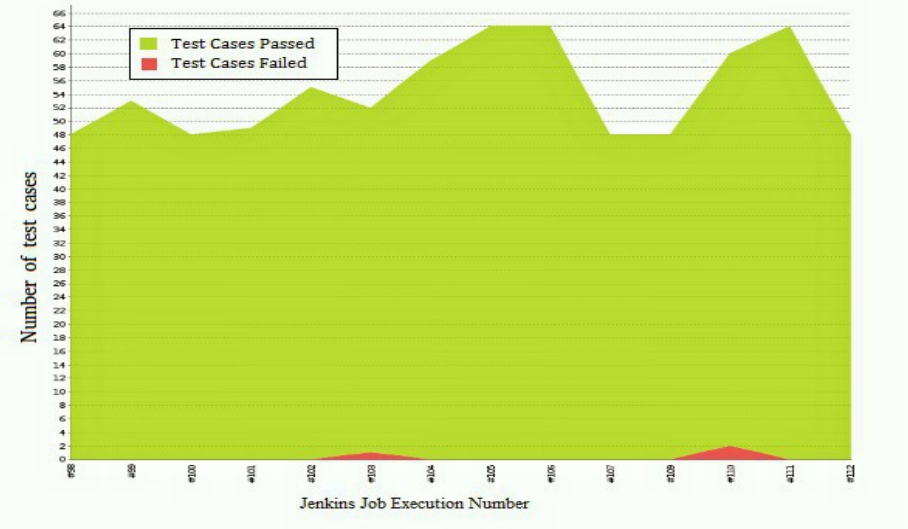


Figure 7.6: Success-Failure trend graph

D. Trend Graph

Trend Graph shows a general trend of success and failures of the builds. The greater the red area, the greater the failure. This type of graph provides a visual effect of the success ratio of the builds. Figure 7.6 shows an example of a success-failure trend. This graph has been plotted for total number of test cases in a particular Jenkins job. Each Jenkins job is triggered with periodically or whenever EnsembleMD or RepEx source code changes are pushed on to the Github.

E. Code Format

Code formatting of any specific language should be ubiquitous. A properly formatted code is easy to distribute, understand and is universally accepted. Our continuous integration system uses Pylint to check the Python code formatting using standard PEP 8 (Style Guide for Python Code). Pylint checks the code-line length, checks for proper spacing, checks if imported modules are used, etc. Figure 7.7 shows the graphical view of violations in the code formatting. The red section in the graph represents a higher priority of violations which needs to be resolved before any product release. Medium and Low violations have less priority and can be ignored as they include unused modules or spacing issues. Figure 7.8 shows an example of the detailed report of the violations with low, medium and high priorities. The report also shows the exact location and reason for the violation.

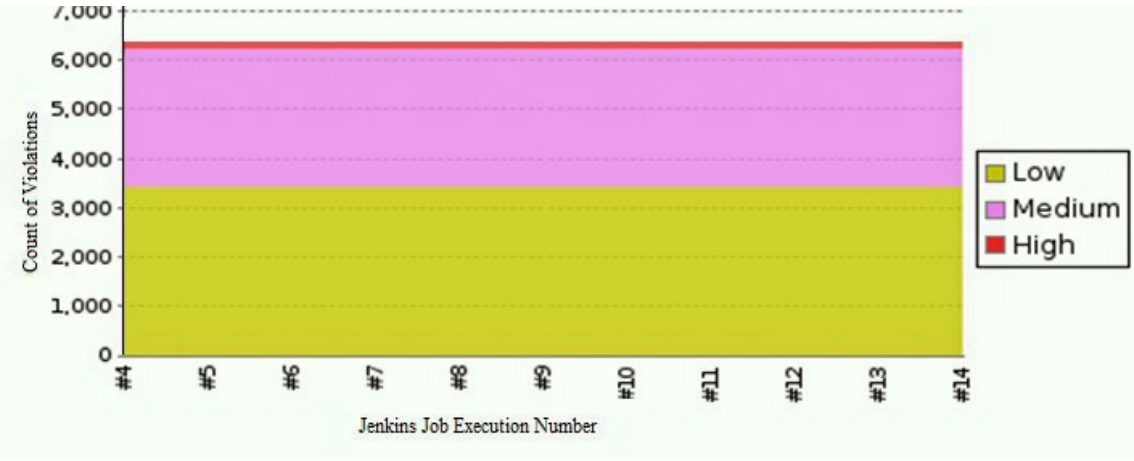


Figure 7.7: Code Format Violations

filename	l	m	h	number ↑
src/radical/ensemblemd/exec_plugins/pipeline/static.py	400	1184	88	1672
usecases/cdi_replica_exchange/replica_exchange_mode_1.py	82	235	8	325
usecases/extasy_gromacs_lsdmap_adaptive/01_static_gromacs_lsdmap_loop.py	210	58	24	292
src/radical/ensemblemd/single_cluster_environment.py	72	183	9	264
usecases/extasy_gromacs_lsdmap_adaptive/misc_files/lsdm.py	134	86	14	234
src/radical/ensemblemd/exec_plugins/replica_exchange/static_pattern_2.py	157	42	24	223
src/radical/ensemblemd/exec_plugins/replica_exchange/static_pattern_3.py	144	46	10	200
examples/tutorial/replica_exchange_b.py	126	52	18	196
usecases/extasy_gromacs_lsdmap_adaptive/misc_files/run.py	118	36	0	154
src/radical/ensemblemd/exec_plugins/replica_exchange/static_pattern_1.py	105	25	22	152
usecases/extasy_gromacs_lsdmap_adaptive/misc_files/reweighting.py	98	32	8	138

Figure 7.8: Code Format Violation Report

Application	**Command**	**Remarks**
Amber	python satlite_exe.py –name “amber” –resource “xsede.stampede” –arguments amber_arguments.wcfg	Single executable example. Tested on Stampede.
CoCo	python satlite_exe.py –name “coco” –resource “xsede.stampede” –arguments coco_arguments.wcfg	Single executable example. Tested on Stampede.
Gromacs	python satlite_exe.py –name “gromacs” –resource “xsede.stampede” –arguments gromacs_arguments.wcfg	Single executable example. Tested on Stampede.
LSDMap	python satlite_exe.py –name “lsdmap” –resource “xsede.stampede” –arguments lsdmap_arguments.wcfg	Single executable example. Tested on Stampede.
Hello World	python satlite_exe.py –name hello –resource xsede.stampede –exe “icpc”,“ibrun” –arguments “hello_test1.wcfg”,“hello_test2.wcfg”	Hello world example with multiple executable. Two executable for compiling and executing c++ hello world program. Tested on Stampede.

Table 7.3: Example of SATLite testing scientific tool

Chapter 8
Conclusion and Future Work

8.1 Conclusion

In this thesis, we attempted to address the issue of HPC resource wastage by minimizing the errors right from the development phase of an application. This thesis pivots around detecting the errors in the ongoing development of scientific tools such as RADICAL EnsembleMD and RepEx. It provides a continuous testing framework to test EnsembleMD toolkit and RepEx frameworks which serve as an abstraction tool for MD simulation packages. The intensive study for this thesis focuses on setting up a 3-stage automatic testing and error reporting framework, the three stages being development, deployment and run-time. As reported by several researchers, a large amount of HPC resource is wasted due to system failures. Their studies mainly concentrated on techniques to curtail the errors from a supercomputers' perspective. The study in this thesis provides a solution to combat the errors at the application level. Mining and analyzing the system logs is a universal approach to developing tools which can automatically detect the error and generate failure reports with proper justification. The logs from the supercomputers do not provide sufficient information to perform automatic detection of failures. Moreover, the system logs do not provide a real-time status of the application. We have used console logs to detect various parameters such as job id or errors or exit codes.

The unit testing and end-to-end testing for EnsembleMD and RepEx covered the important APIs and functionalities to check the software and implementation bugs. These toolkits were continuously tested by the Jenkins CI server, hence ensuring their stability. We observed that the test cases we developed could successfully test the proper functioning of EnsembleMD and RepEx and capture the errors in their source code. The development level testing can help in fixing the software bugs right in the development phase. The SATLite tool is able to capture deployment and run-time errors when scientific tools are executed directly on to the supercomputers. This error reporting can help molecular dynamics community and developers to achieve confidence in their simulation packages. This testing suite was able to capture code bugs and logical errors in EnsembleMD and RepEx tools. At deployment and run-time phases, SATLite was able to capture environment setup failures, errors

due to obsolete modules, input file errors, execution failures or even improper execution.

8.2 Future Work

There is a broad scope in the development of error detection tools to enhance the performance of applications on supercomputing resources. An ideal bug-free application should be tolerant to any system upgrades or changes and should have optimized execution to utilize the maximum performance of supercomputers. As the scientific tools are continuously updating, so are EnsembleMD and RepEx. There is always an opportunity to increase the number of test scenarios to check the source code bugs and to establish a confidence in the application.

The SATLite tool has been currently developed for SLURM job schedulers and tested on Stampede supercomputer. In future scope, SATLite has to be extended for resources with other job schedulers such as PBS. To achieve this, one of the approaches could be to use RADICAL SAGA [20],[26] as an underlying framework as it can handle a large number of job schedulers and batch scripts. Moreover, error detection can be improved by translating exit code to text-based reporting. A more intensive usage of SATLite with many scientific applications can help in expanding this testing framework. The proof-of-concept of SATLite proves to be promising in minimizing the application failures due to software bugs or improper environment loading or incorrect input files. It can be used by the developers and scientists to scrutinize their application before actually releasing it for their users.

8.3 Links to Current Work

The current development version of the testing framework can be downloaded from the below mentioned Github links.

- **EnsembleMD Unit Testing:** https://github.com/suvigya91/EnsembleMD-Testsuit
- **RepEx Unit Testing:** https://github.com/suvigya91/repex-test
- **SATLite- Deployment and Run-time testing suit:** https://github.com/suvigya91/SATLite
- **SATLite readthedocs:** http://satlite.readthedocs.io/en/latest/
- **Jenkins CI server:** 144.76.72.175:8080

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