Title	Change Request Analysis Internal Document	
Version	2.0	1.0
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Date	17/02/2023	
Comments	This is the analysis for the first change request on the LJ MD system	

Change Request Analysis Internal Document

Introduction

This document outlines the results of a change request analysis conducted for the Lennard Jones simulation system, as proposed by our clients. The system design includes a numerical algorithm, namely the Velocity-Verlet algorithm, which is used to solve the dynamic equations for an ensemble of particles interacting with a central potential. **The clients expressed their interest in expanding the capabilities of the system for solving a variety of differential equations.**

In the following sections of this document, we analyze the change request (CR) from several fundamental perspectives that are essential for the overall development of the project.

Configuration items

The first step in every configuration management (CM) process is to analyze the configuration items (CIs). In this document, we will use the following definition for CIs:

"A configuration item is a module, or part of a system that needs to be modified in order to meet the needs of a change request (CR)"[1]

However, we have encountered a different definition in the literature that extends the term further, taking it out of the context of CRs. For example:

The term **configuration item** or **CI** refers to the fundamental structural unit of a configuration management system. Examples of CIs include individual requirements documents, software, models, and plans.*

And:

[1] Class definition?

A configuration (configured) item is defined as any product that requires formal release and control of supporting information prior to acceptance by the user; where the supporting information is detailed with sufficient precision for all internal and external stakeholders to understand.

These definitions were taken from (Quigley & Robertson, 2019).

We consider three modules for our original system:

- GUI
- Simulation module
- Output module

For assessing the impact of a CR on a given module we consider the following criteria:

1. Functionality: to evaluate if implementing a CR would require to add, remove or modify the existing functionality of a module.
2. Data: to asses if the type of data that the module receives, outputs or processes is compatible with the needs of the CR.
3. Performance: to asses if the predefined computational resources of the system will suffice the CR's computational intensity.
4. Dependencies: to check if he module depend on other modules or components that may be affected by the change request.
5. Documentation: to check if the request require modifications to the existing documentation or the addition of new documentation to reflect the changes made to the module.

Configuration items

Under the above criteria we have encountered that all the modules in our system would be identified under the first definition as CIs as described in the following table.

CI-ID	Name	Criteria
CI01	GUI	1, 2, 4, 5
CI02	Simulation module	1, 2, 3, 4 ,5
CI03	Output Module	1, 2, 4, 5

Technical analysis

The range of applications of differential equations (DEs) varies enormously, from modeling the stock market to describing the quantum behavior of an electron. Consequently, DEs are highly diverse and varied. Therefore, the idea of a universal method that can solve all types of DEs is inspiring, but it is currently beyond our capabilities.

The Lennard Jones simulation system was designed to solve a specific, well-defined mathematical problem. The algorithm used for numerical analysis is well-known, but it is

mathematically constrained to systems of second-order differential equations, making it infeasible to use it beyond this scope. Therefore, in order to satisfy the needs of our clients, we would have to invest a significant amount of time investigating and implementing other methods for computing solutions to differential equations, such as the finite element method, Euler's method, and series methods. **We belive that the only component that would remain from the original system would be the numerical integrator, hence, going this way would imply to change more than 90% of the project, taking it out of scope.**

Although the system we proposed can be adapted to solve other classical mechanics problems, such as the dynamics of celestial bodies, additional work would need to be done to simulate more complex molecular systems, such as liquid crystal-like molecules or mixtures.

The technical analysis committee emphatically states that the clients should be oriented and guided towards identifying their real needs, and that a common ground should be established to continue with the project. **We believe that solving differential equations is not a business need in itself, and we must understand what applications the clients have in mind for these computations in order to offer them a viable solution.**

Financial analysis

The original budget for the project was planned to be used over the six-month period covering the implementation, testing, and deployment phases. However, it has been found that the budget is sufficient to cover the expenses of the team for nine months, assuming the same expense rate is maintained.

This project is considered a top priority in our portfolio. However, as stated in the technical analysis, whether to continue with the project depends entirely on the clear identification of the client's needs and their willingness to update the budget. **Failure to continue with the project could compromise the company's finances, as it would result in an expected net profit decrement of 30% this year.**

The financial analysis committee strongly recommends continuing with the project, provided that it is profitable. Nonetheless, further analysis needs to be carried out by the remaining committees.

PR analysis

The PR analysis committee recognizes the high value of the clients involved in this project, as they may represent the opportunity to expand our client base in the scientific software market. Regarding the small and competitive nature of this market, our market**, we recommend continuing with the project even if it involves a net financial cost to the enterprise. By building a strong relationship with these clients, we can potentially secure long-term revenue and solidify our position in the market**. It is important to communicate

the value of this project and the potential benefits to the company to both the financial analysis committee and the clients themselves.

The PR committee suggests creating a sales group to promote the Lennard Jones simulation software product to new companies. This would help mitigate the financial stress the company might face by continuing with this client.

Note

Further analysis of infrastructure and human resources requirements must be deferred until the clients' needs are clearly defined and the management team has decided on whether to proceed with the project or not.

Metrics: criteria and scales

Technical analysis

Metric name	Low	Medium	High
Code coverage risk	Below 20%	20%-50%	Above 50%
Technical Debt	Below 10% of available time	10%-20% of available time	Above 20% of available time

Financial analysis

Metric name	Low	Medium	High
Net revenue risk	Below 20%	20%-50%	Above 50%
Return time risk	Before 12 months	12-18 months	After 18 months
Return of investment	Below 10%	10% -20%	20%

PR analysis

Metric name	Low	Medium	High
Referral rate (with respect to current number of clients)	Below 10%	10%-20%	Above 20%
Probability of repeat	Below 30%	30-60%	Above 60%

Bibliography

- Quigley, J. M., & Robertson, K. L. (2019). *Configuration management: Theory, practice, and application*. Auerbach.