

Project Directive

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Version 1.0

Status

Reviewed		
Approved		

PROJECT IDENTITY

Linköping university, IFM

Group members

Name	Responsible	E-mail
	Project manager	
	Documents	
	Code Design	
	Code Test	
	Code Implementation	
	Program Operation	

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Contents

1. INTRODUCTION
2. OVERVIEW OF THE PROJECT
3. DESIGN AND FLOW OF THE MD PROGRAM
4. PERFORMANCE REQUIREMENTS
5. UPGRADE CAPABILITIES
6. RELIABILITY
7. DELIVERY
8. DOCUMENTATION
9. EDUCATION
10. REFERENCES

Document history

Version	Date	Changes	Sign	Reviewed
1.0	25 Aug 2009	Customer requirement specification		

1. Introduction

This document describes the design requirement specification for an operational Molecular Dynamics (MD) computer program. The MD code could be written in any of the common programming languages and is intended to simulate the behaviour of materials found in nature. The end result will be a program able to reproduce the *real* laws of physics at the microscopic level so it can be used for realistic predictions in the design of new materials.

1.1 Involved Parties

The following parties are involved in this project: the customer, the project leaders, the project members, the supervisor and experts. The project supervisor acts as a customer and the main project leader. He assigns the project leaders and follows the project course, he formulates the requirements and also reviews the project documents. The assigned project leaders are responsible for realization of the given tasks in smaller groups of project members. The project experts can be consulted by the involved parties during the project period.

1.2 Project Goal

The project goal is to design, implement and operate a Molecular Dynamics (MD) program. Students participating in this project as project members and project leaders should learn the different steps of the MD coding design flow, analyse results obtained with the program and assert the quality of the results. That includes the correct selection and writing of code subroutines, MD program assembling, compiling, debugging and testing, and finally operating the program. The project students have an optional choice to add visualization capabilities to the MD code, which would help in understanding and analysing microscopic processes simulated with MD.

1.3 Usage

The MD program is intended for academic use and it should reliably simulate and calculate materials behaviour and properties. The experience gained in this project could be reused to fully operate and/or develop more complex industrial/academic software used in materials science.

1.4 Available resources

- Scientific software
 - MD subroutines available (Fortran only).
- Scientific publications database
- Software & Hardware Tools
 - Materials Studio Modelling
 - Matlab
 - Dedicated hardware (4 x Windows/XP machines) & SUN workstations.

2. Overview of the project

2.1 Project parts

The main parts of the project are:

- Conceive and design a MD program for a specific class of materials
- Implement the MD code and test the quality of the MD simulations

- Operate the MD program to calculate additional properties and assess the results

2.2 Project stages

There are three important stages in this project:

1. Successful finalisation of the MD computer program.
2. Quality assessment of the MD methodology implemented.
3. Material properties prediction/calculation and analysis of results obtained.

3. Design and flow diagram of the MD program

Typically, MD programs are designed based on the type of problems that will be studied, i.e. the choice of the design is based on the material class for which they will be used. Accordingly, the flow diagrams of the MD programs reflect this initial choice. The design and flow diagrams of the MD programs in the project will have to correctly reflect these essential criteria.

4. Performance requirements

The table below summarizes the basic performance requirements of a MD program. With each requirement, a degree of priority is associated.

Req. 1.	Initial MD system set up (atomic configuration, MD parameters, periodic boundary conditions, neighbour lists etc)	High
Req. 2.	Interaction Potential definition and parameterisation (based on material class).	High
Req. 3.	Integrator of equations of motion	High
Req. 4.	Efficient force calculation (analytic or tabulated)	High
Req. 5.	MD step set up (including correct calculation of bulk material properties: cohesive energy, temperature, pressure)	High
Req. 6.	Additional routines for calculation of other important material properties (diffusion constant, bulk modulus etc)	Low/ Extra

5. Upgrade capabilities

An important part of this project is to learn how to operate the software.

Req. 7.	The MD program should be easily upgraded and able to simulate surface processes	Low
Req. 8.	Visualization capabilities would be an extremely useful addition and/or upgrade of the MD code	Optional

6. Reliability

The MD program should reliably reproduce the microscopic processes upon which important material properties can be calculated. If this is achieved, i.e. if known properties are simulated

correctly, the program can then be used to make accurate predictions for that class of materials, an instrumental part of industrial/academic current materials science research.

7. Delivery

The MD program will be tested during the project. A description of the program, together with the results of simulations, will be included in a final report, to be presented to the supervisor.

8. Documentation

The project status must be documented according to the project plan. All documentation will be presented in the LIPS v1 format. Document templates will be available from the supervisor. The following documents will be required in this CDIO project:

- requirement specification
- project plan
- time plan
- final report; this will include program description, analysis of results and comparison with experiments.

A reflection document, in which project participants are required to evaluate their own work, as well as the course and project, will also have to be prepared.

9. Education

To facilitate the MD program design process, lectures and laboratory exercises will be offered mostly before the actual project will begin.

10. References

Svensson, T, Krysanter C. (2002). The compendium LIPS –nivå 1 version 1.0