**MPhys Draft Report**

**1 Introduction**

It is well known that deoxyribonucleic acid (DNA) is one of the most important substances in all life on Earth. DNA encodes all the instructions required for an organism to function. The language of the instruction is composed of four basic units (cytosine C, thymine T, . These instructions are capable to be passed , thanks to a

Despite a majority of the genetic information of life is stored in the DNA, over the past few decades scientists have discovered that some modifications. These heritable changes in genes which do not involve alterations in the genetic sequence of the DNA are referred as epigenetic (cite DNA book, probst2009). Different classes of epigenetic modifications have been identified. For instance, these could be direct biochemical modifications on the nucleotides (e.g. DNA methylation) or histone proteins, which are prot. These modifications are important as they

A major focus in the study of epigenetics is to understand the mechanisms behind the establishment of epigenetic patterns and the stable inheritance of these modifications over generations of cells.

A class of approach used to understand the mechanisms is through mathematical modelling. Many biophysical models have been proposed and used to investigate epigenetic modifications and have successfully explain some aspects of establishment and inheritance of epigenetic marks. However, most of these models focus only on the epigenetic landscape. It has long been recognised that there are interconnections between chromatin dynamics and epigenetic modifications (cite). Hence, it would be important . In addition, a lot of the models only allow the proliferation of a single epigenetic mark on the modelled chromatin. It is clear that for information to be . Hence, it is important to develop a model t

The project focuses on investigating the coupling of another

coupling a stochastic one-dimensional model proposed by Dodd et. al. (cite), which successfully characterise the spreading and maintenance of epigenetic marks, with a three-dimensional polymer model that describes chromatin dynamics. The epigenetic model proposed by Dodd et. al. based . Like the

The remaining sections of the report are as follows: Section 2 provides an overview o

**2 Background**

**Epigenetics**

The research on epigenetics has come a long way since Waddington first proposed the term in 1970s. Many forms of epigenetic modifications have been identified along with their functions

Different classes of epigenetic marks.

Focus on histone/nucleosome modification

**Histone Modifications as Epigenetic Marks**

**Correlation between Epigenetic Modification and Chromatin Dynamics**

**A Stochastic Model for Nucleosome Modification**

**3 Methodology**

**Simulation Model**

In the project, we simulated a chromatin fibre as a semi-flexible “bead-and-spring” polymer of N beads. In line with common mappings employed in modelling chromatin dynamics [cite], each bead represents roughly 3 kbp, which corresponds to around 15 nucleosomes. Each bead

The interactions be

The epigenetic modification is based on the model proposed by Sneppen et. al.

The modification is coupled to the chromatin dynamics.

The m

**Initialisation Procedure**

As in any molecular dynamics simulation, it is important to describe the initialisation procedure. The initial state of the chromatin fibre used in each simulation is created based on the random walk model. Each

**Program Structure and Software Used**

**Testing**

**Results**