

YOUR TITLE GOES HERE

By

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A thesis submitted in partial fulfillment of  
the requirements for the degree of

BACHELOR OF SCIENCE

UNIVERSITY OF THE PHILIPPINES - DILIMAN  
National Institute of Physics

FEBRUARY 2020

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To the Faculty of Washington State University:

The members of the Committee appointed to examine the thesis of CHRISTIAN LOER  
T. LLEMIT find it satisfactory and recommend that it be accepted.

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## ACKNOWLEDGMENT

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Abstract

by Christian Loer T. Llemit, Ph.D.  
University of the Philippines - Diliman  
February 2020

: Rudyard Kipling

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## **Dedication**

This dissertation/thesis is dedicated to my mother and father who  
provided both emotional and financial support

# Chapter One

## SOME FORMATTING EXAMPLES

### 1.1 Chapter one tittle section

#### 1.1.1 Subsection of section - double quotes

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#### 1.1.2 Another subsection of section - citations

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Example of multiple citations (Altschul et al., 1997; Baker et al., 2007). Nullam mollis et leo at pharetra. Nulla efficitur molestie euismod. Sed dapibus metus sed tempus varius. Aenean finibus eros ut urna luctus feugiat. Duis turpis risus, viverra vitae porta et, ullamcorper ac est. Proin in eros nec ipsum interdum tempus. Nam fringilla lectus velit, non posuere ex vehicula ut. Mauris tincidunt, dolor sit amet commodo tempor, erat mi egestas dui, at elementum tellus est rhoncus libero. Ut et rutrum lectus, id viverra tortor. Vivamus nec lacus eros. Donec dictum porta nisi et vestibulum. Mauris luctus ligula ut libero aliquet luctus. Quisque malesuada egestas finibus.

#### **1.1.2.1 Subsubsection of section - italic text**

Example of italic text - *Escherichia*, *Salmonella*, and *Shigella* spp. Mauris dictum pharetra fermentum. Maecenas ut felis varius, dapibus sapien imperdiet, dictum dui. Proin feugiat viverra metus non laoreet. Integer pulvinar mi id lacus semper commodo. Praesent vel erat interdum purus scelerisque maximus. Sed enim risus, mollis blandit ligula ac, sagittis venenatis augue. Mauris nisi purus, gravida ac aliquam eu, ullamcorper eget nulla. Proin id finibus purus. Vestibulum leo ante, porta in quam sed, eleifend feugiat arcu. Nunc viverra fringilla turpis a iaculis. In condimentum aliquet mauris, quis laoreet eros porta eu. Aenean ut turpis a massa gravida pretium. Phasellus auctor purus quis diam interdum, nec luctus lorem auctor. Pellentesque finibus elit justo, a vulputate diam fermentum lacinia.

## 1.2 Another section

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## 1.3 Another section

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# Chapter Two

## LINKS

### 2.1 Chapter one tittle section - links examples

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### 2.1.1 Subsection title - more links examples

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## 2.2 Another Section

### 2.2.1 Subsection title

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# Chapter Three

## INTRODUCTION TO MY THESIS

### 3.1 ME MYSELF AND I

#### 3.1.1 Subsection of section - double quotes

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# Chapter Four

# THEORETICAL FRAMEWORK

## 4.1 Quantum Mechanics

### 4.1.1 Simplifying Assumptions

### 4.1.2 Time Independent Schrödinger Equation

### 4.1.3 Use of Atomic Units

### 4.1.4 Hamiltonian Operator

### 4.1.5 Indistinguishability of electrons

## 4.2 Early First Principle Calculations

### 4.2.1 n-electron problem

### 4.2.2 Hartree Method

### 4.2.3 Hartree-Fock Method

## 4.3 Density Functional Theory

### 4.3.1 Electron Density

### 4.3.2 Hohenberg-Kohn (HK) Formalism

#### 4.3.2.1 First HK Theorem

#### 4.3.2.2 Second HK Theorem

### 4.3.3 Kohn Sham (KS) Formalism

#### 4.3.3.1 KS Equation

#### 4.3.3.2 Energy Terms

# Chapter Five

## DFT Calculation of Solids

### 5.1 Pseudopotential Approach

This is sample text

5.1.1 Freezing the core electrons

5.1.2 Pseudizing the valence electrons

5.1.3 Common Pseudopotentials

## 5.2 Choosing the appropriate Calculation Size

5.2.1 Use of Supercell

5.2.1.1 Periodic Boundary Conditions (PBC)

5.2.2 Use of Reciprocal Space

5.2.2.1 Reciprocal Lattice

5.2.2.2 First Brillouin Zone

5.2.2.3 Irreducible Brillouin Zone

5.2.3 k-point sampling

5.2.3.1 Monkhorst-Pack method

5.2.3.2 Gamma Point Sampling

Example of double quotes “word”. Lore





## 5.3 Bloch Representations

### 5.3.1 Electrons in solid

### 5.3.2 Bloch Theorem in periodic systems

### 5.3.3 Fourier Expansion of Bloch representations

#### 5.3.3.1 Fourier Expansions

#### 5.3.3.2 Fast Fourier Transformation (FFT)

#### 5.3.3.3 Kohn-Sham Matrix Representations

## 5.4 Plane Wave (PW) Expansion

### 5.4.1 Basis Set

#### 5.4.1.1 Local Basis Set

#### 5.4.1.2 Plane Wave Basis Set

### 5.4.2 Plane Wave Expansion for KS quantities

#### 5.4.2.1 Charge Density

#### 5.4.2.2 Kinetic Energy

#### 5.4.2.3 Effective Potential

## 5.5 Electronic Structure

### 5.5.1 Band Structure of free electrons

### 5.5.2 Band Structure of electrons in solids

### 5.5.3 Electronic Density of States

## 5.6 Practical Aspects

# Chapter Six

## MATHEMATICS NOTATION

### 6.1 Some Math Stuff

LaTeX has a special way to embed mathematical symbols and notations. Here are some of them. Also observe how a bullet list is made.

- greater than  $\geq$
- less than  $\leq$
- percent sign %
- multiply  $N \times N$
- inline equation  $M = N(N - 1)/2$

Sed orci justo, rutrum in dolor a, consequat dictum mi. Sed luctus congue ex nec dignissim. Phasellus volutpat urna vestibulum ipsum vestibulum, quis venenatis justo consectetur. Nullam hendrerit nisl in rutrum convallis. Sed sit amet malesuada nisi. Phasellus dolor neque, vehicula vestibulum semper at, facilisis eget libero. Mauris interdum magna molestie, auctor felis a, condimentum odio. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Suspendisse maximus lacinia dignissim. Maecenas pharetra accumsan metus, sagittis dictum purus sollicitudin eget. Curabitur ut porttitor arcu, ut porttitor ipsum. Vestibulum porttitor finibus sapien, ac pharetra odio bibendum nec. Nullam tincidunt dignissim risus imperdiet dictum.

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## 6.2 Math equation

Example of a mathematical formula:

$$ADD = \sum_{i=1}^M | < D(n+1, i) > - < D(n, i) > | \quad (6.1)$$

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## 6.3 Chapter section

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## 6.4 Chapter section

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# Chapter Seven

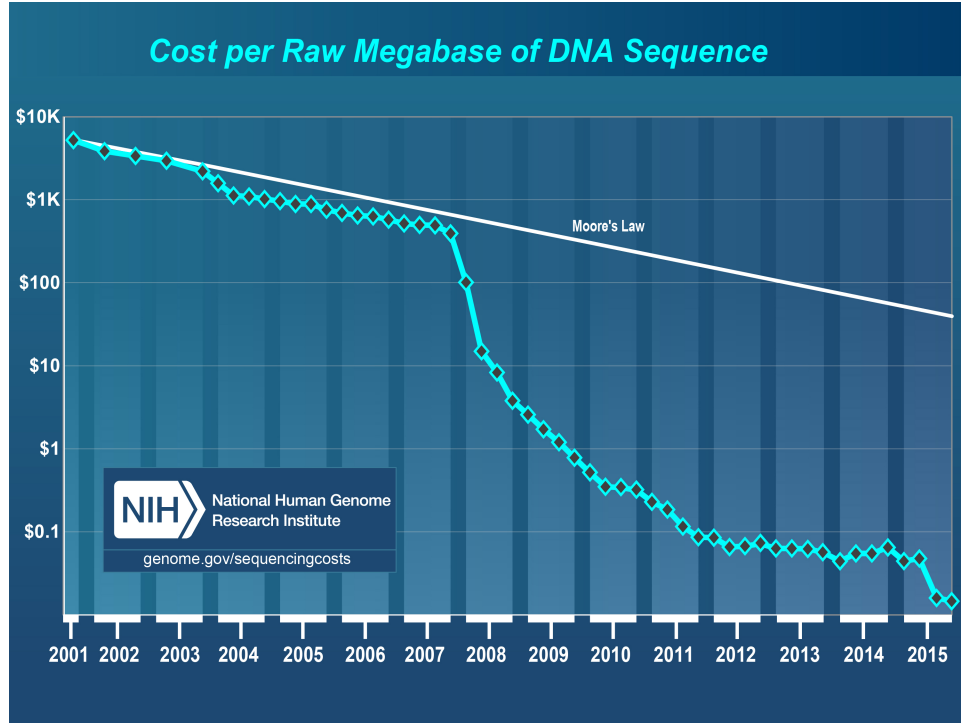
## FIGURES AND TABLES

### 7.1 Examples of a figure

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Example of a figure. Example of reference to a figure in the text (Fig. 7.1). Phasellus dolor neque, vehicula vestibulum semper at, facilisis eget libero. Mauris interdum magna molestie, auctor felis a, condimentum odio. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Suspendisse maximus lacinia dignissim. Maecenas pharetra accumsan metus, sagittis dictum purus sollicitudin eget. Curabitur ut porttitor arcu, ut porttitor ipsum. Vestibulum porttitor finibus sapien, ac pharetra odio bibendum nec. Nullam tincidunt dignissim risus imperdiet dictum.

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**Figure 7.1** Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore’s Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from (Wetterstrand, 2016)

## 7.2 Example of a table

Example of a table and here is the reference to Table 7.1. Tables in, my opinion, are the hardest thing to make.

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ORGANISM	ACCESSION NO.	GENOME SIZE (bp)	No. CDS
<i>Mesorhizobium loti</i>	NC_002678	7036071	6743
<i>Sinorhizobium meliloti</i>	NC_003047	3654135	3359
<i>Bradyrhizobium japonicum</i>	NC_004463	9105828	8317
<i>Rhodopseudomonas palustris</i>	NC_005296	5459213	4813
<i>Bartonella quintana</i>	NC_005955	1581384	1142
<i>Bartonella henselae</i>	NC_005956	1931047	1488
<i>Rickettsia typhi</i>	NC_006142	1111496	837
<i>Beijerinckia indica</i>	NC_010581	4170153	3569

**Table 7.1** Whole-genome sequences used in this study

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## 7.3 Chapter section

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maximus lacinia dignissim. Maecenas pharetra accumsan metus, sagittis dictum purus sollicitudin eget. Curabitur ut porttitor arcu, ut porttitor ipsum. Vestibulum porttitor finibus sapien, ac pharetra odio bibendum nec. Nullam tincidunt dignissim risus imperdiet dictum.

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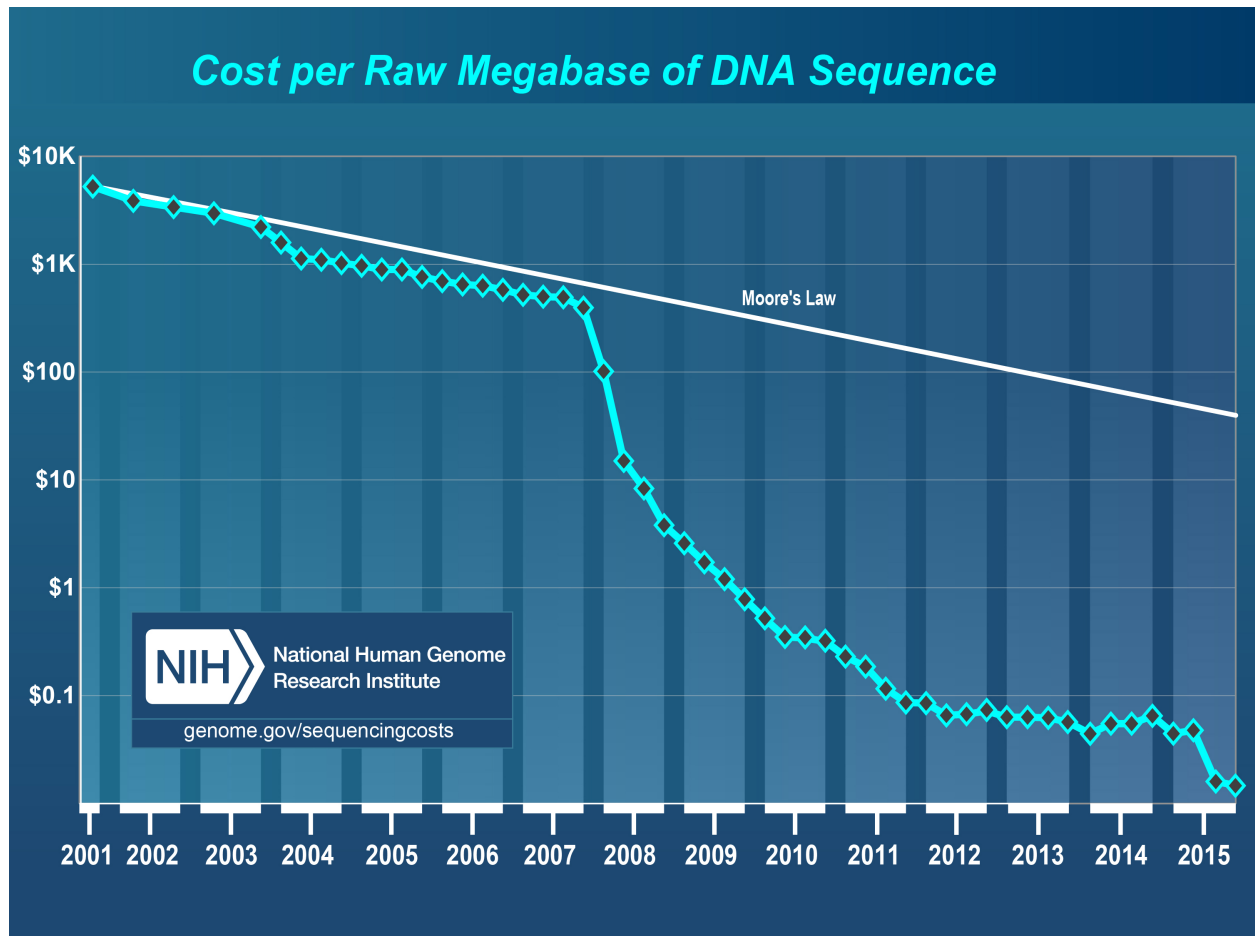


# REFERENCES

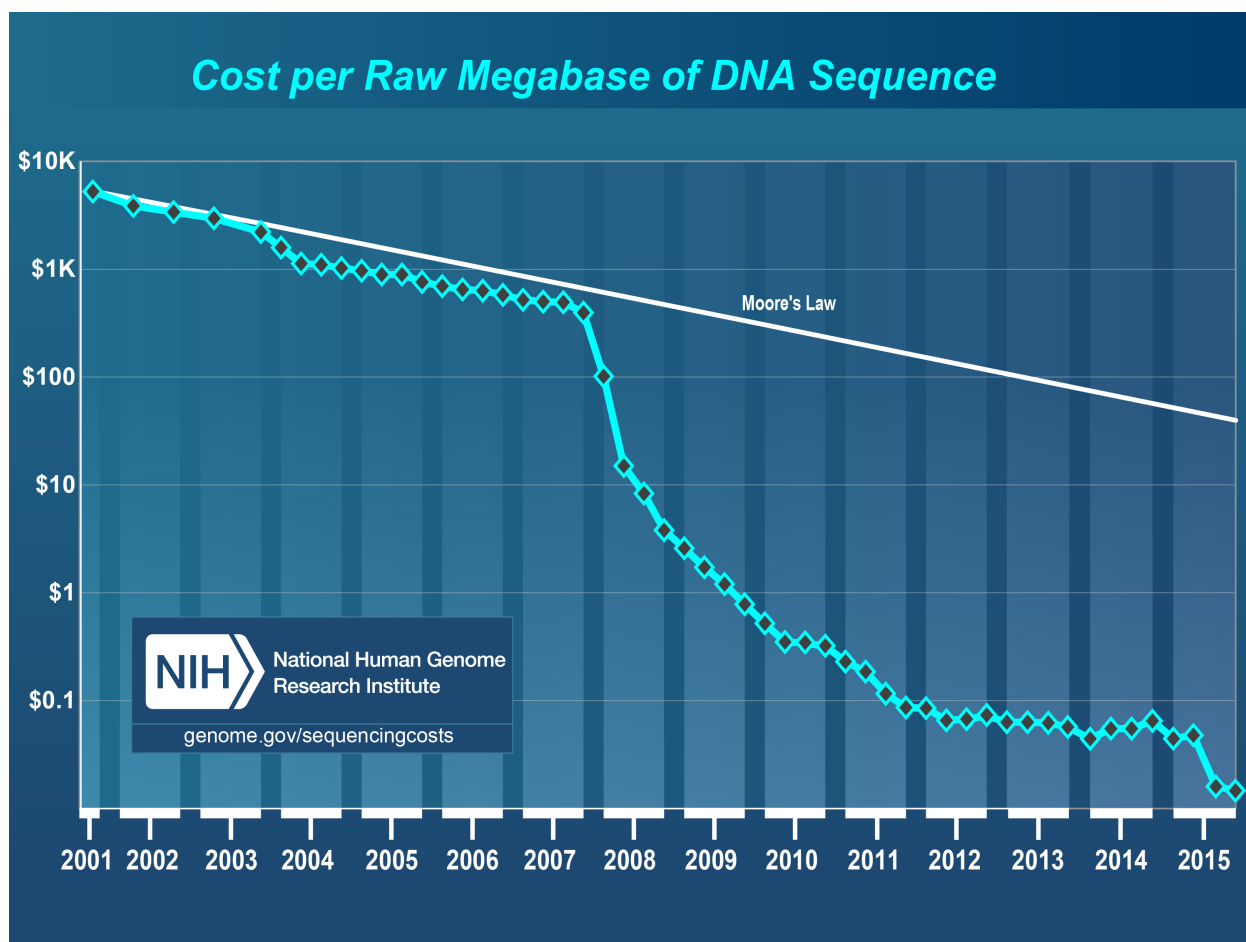
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- Baker, Stephen et al. (2007). “A novel linear plasmid mediates flagellar variation in *Salmonella* Typhi”. In: *PLoS Pathog* 3.5, e59.
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## APPENDIX

# Appendix A

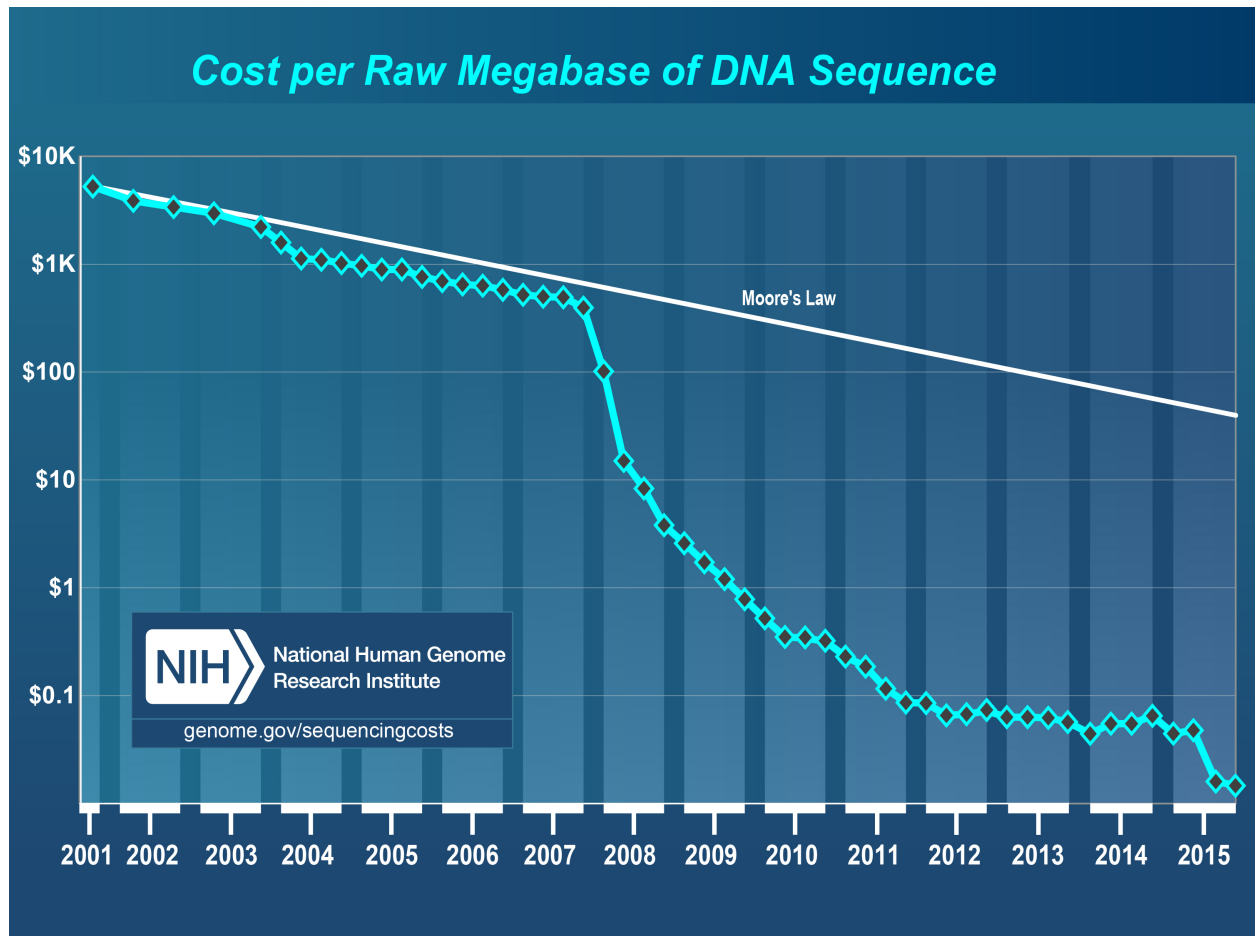


**Figure A.1** Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from (Wetterstrand, 2016)



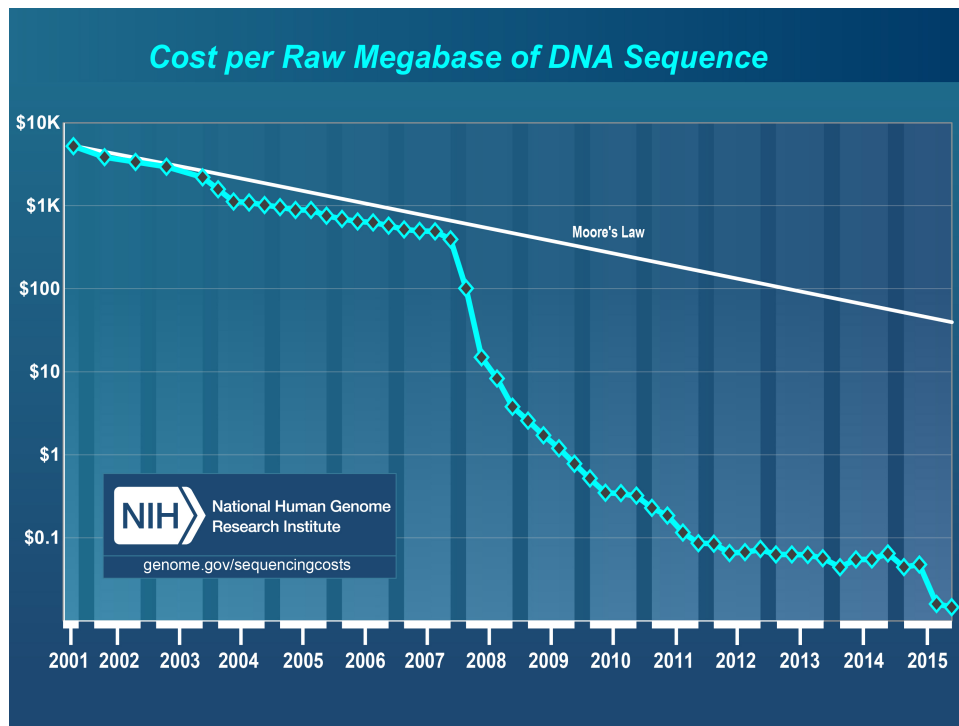
**Figure A.2** Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from (Wetterstrand, 2016)

## Appendix B



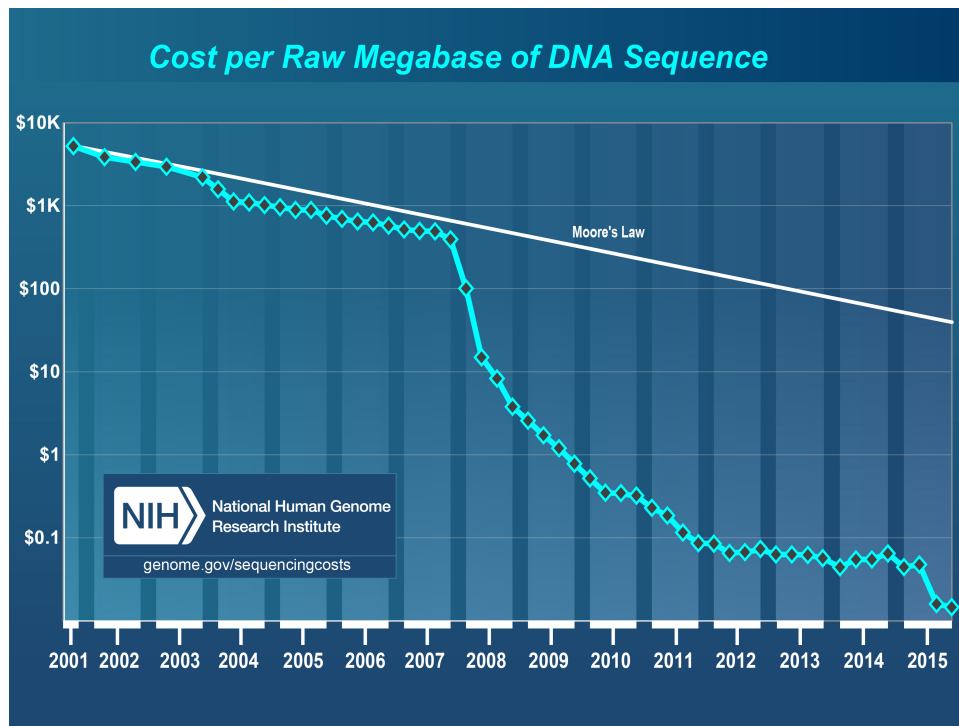
**Figure B.1** Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from (Wetterstrand, 2016)

## Appendix C



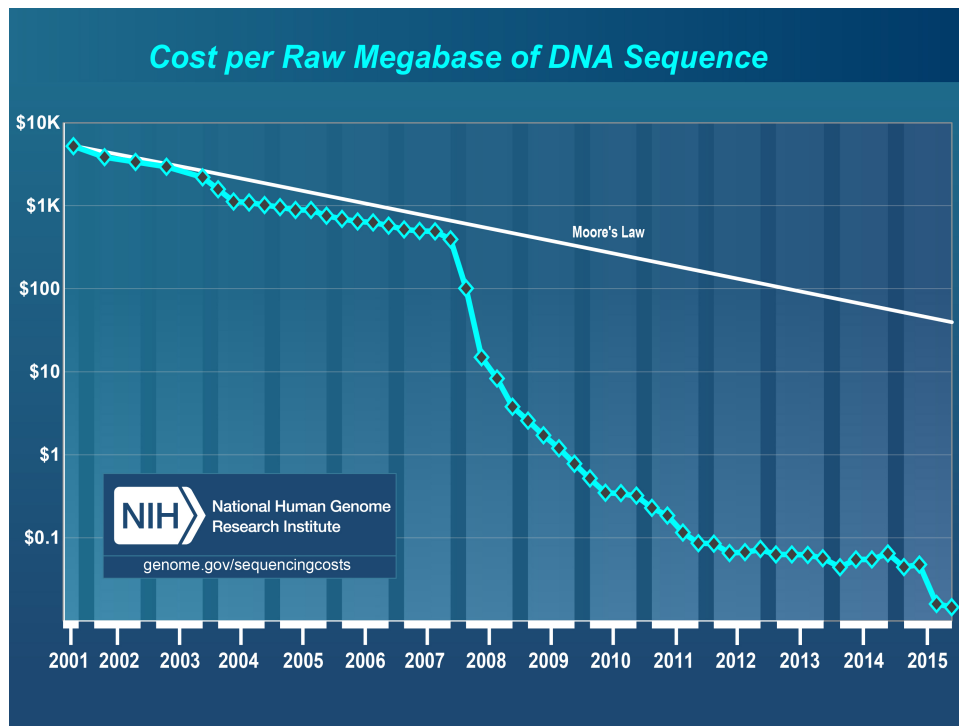
**Figure C.1** Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from (Wetterstrand, 2016)

## Appendix D



**Figure D.1** Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from (Wetterstrand, 2016)

# Appendix E



**Figure E.1** Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from (Wetterstrand, 2016)