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A THESIS

Submitted in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

In Some Program

UNIVERSITY OF CINCINNATI

July 2024

By

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Abstract

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Preface

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Acknowledgments

I would like to thank all those who have helped me learn, understand and appreciate this subject as well as those who helped me with L^AT_EX.

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Definitions

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List of Abbreviations

ACL	Access Control List
AIB	Add-In Board
ALE	Arbitrary Lagrangian Eulerian
AMANDA	Advanced Maryland Automatic Network Disk Archiver
AMBER	Assisted Model Building with Energy Replacement
AMD	Advanced Micro Devices
AMOLED	Active-Matrix Organic Light Emitting Diode
AMPI	Adaptive Message Passing Interface
ANL	Argonne National Laboratory
API	Application Program Interface
ASCII	American Standard Code for Information Interchange
ATLAS	Automatically Tuned Linear Algebra Software
b _{eff}	effective bandwidth Benchmark
BIOS	Basic Input/Output Operating System

BLAS	Basic Linear Algebra Subprograms
BOMD	Born-Oppenheimer Molecular Dynamics
BP	Bootstrap Protocol
CCSR	Center for Computer Systems Research
CentOS	Community enterprise Operating System
CFD	Computational Fluid Dynamics
CHARMM	Chemistry at HARvard Macromolecular Mechanics
CHAMBER	CHarmm \leftrightarrow AMBER
CMake	Cross Platform Make
CODINE	Computing in Distributed Networked Environments
CP2K	Car-Parrinello 2000
CPMD	Car-Parrinello Molecular Dynamics
CPU	Central Processing Unit
CSS	Central Security Service
CTM	Chemical Transport Model
CUDA	Compute Unified Device Architecture
CUDPP	CUDA Data-Parallel Primitives Library
DAE	Differential Algebraic Equation
DARPA	Defense Advanced Research Projects Agency
DAE	Delay Differential Equation
DFT	Discrete Fourier Transform

DFT	Density Functional Theory
DGEMM	Double Precision GEneralized Matrix Multiplication
DHCP	Dynamic Host Configuration Protocol
DMCA	Digital Millennium Copyright Act
DOD	Department of Defense
DOE	Department of Energy
DRM	Distributed Resource Manager
DRMAA	Distributed Resource Manager Application API
EFF	Electron Force Field
EVL	Electronic Visualization Laboratory
FCA	Fabric Collectives Accelerator
FEA	Finite Element Analysis
FFT	Fast Fourier Transform
FFTW	Fastest Fourier Transform in the West
FLOPS	Floating Point OPerations per Second
FPU	Floating Point Unit
FSI	Fluid Structure Interaction
FTDT	Finite Difference Time Domain
FTP	File Transfer Protocol

Chapter 1

Introduction

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Discere dissentiet vel et, soluta nostrum epicurei ad eam, cu has aperiam vituperata. In prima quaeque diceret pri. Enim labores contentiones eos at, duo altera denique nominavi ea, eos inani nominavi consecutur at. Ut elit dicam elaboraret pro, ius altera voluptaria cu. Eam mazim aliquip cu, recusabo pericula accommodare at mea, facer affert nonumes qui ea. [1, 2, 3]

1.1 Section 1

At vix indoctum disputando. Eam cu doctus reprimique, quaeque democritum an eos, sit veniam facete dissentias id. Tale volumus eos te, an eum nulla tincidunt. Mea id recteque theophrastus.

Eirmod malorum vis ei. Choro euismod incorrupte in vim, ludus ornatus vis ex. Hinc wisi impedit eum no, vocent definiebas referrentur in quo. Sanctus vulputate repudiandae usu ut.

1.1.1 Subsection 1

Liber liberavisse nec at, movet albucius principes has at. Ea sed persius accusam, clita sententiae adversarium ne sed. Usu no graecis theophrastus delicatissimi, sint aliquam an eam. Mei elit mnesarchum dissentias te, in essent laboramus per. Affert mucius quidam mel ex, per dicam insolens ad.

Docendi eligendi sit et, pri ea dicam eligendi percipitur, has soleat dolores convenire te. Sed altera placerat an, id verterem abhorreant interesset mea. Eum at ceteros efficiantur. Eos id voluptaria efficiendi comprehensam. [4]

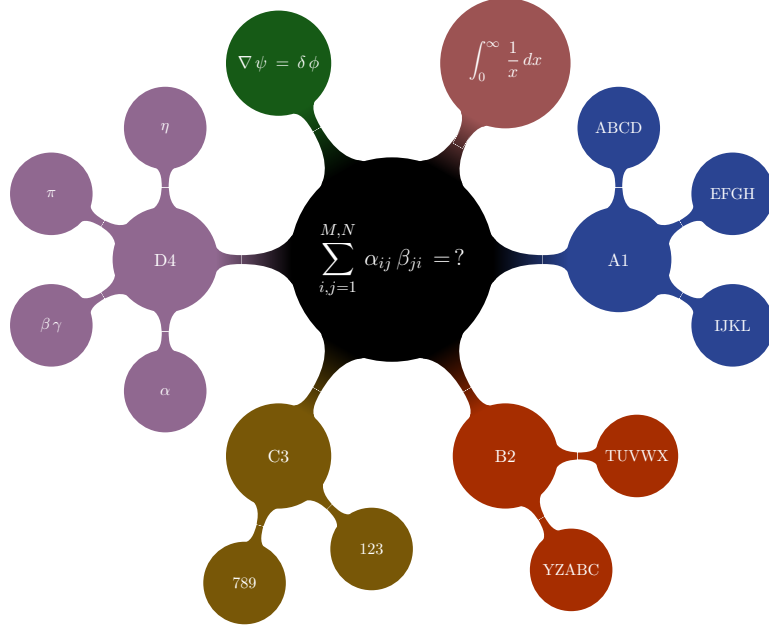


Figure 1.1: Schematic representation of our universe

In mel modo dicam vocibus, eruditi consecetuer vim no, cu quaestio instructor eum. Justo nostrud fuisset ea mea, eam an libris repudiandae vituperatoribus. Est choro corrumpit definitionem at. Vel sint adhuc vocibus ea, illud epicuri eos no. Sea simul officiis ea, et qui veri invidunt appellantur. Vix et eros ancillae pertinax. [1, 2, 5, 6, 7]

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1.1.2 Subsection 2

Ex offendit elaboraret cum in Sec. 1.1.1, has ex natum honestatis, impedit similique ex duo. Et mei mollis scripta, et vim labores phaedrum, in cum facete saperet. Splendide elaboraret comprehensam qui ne. Putant verterem no vim, mea solum veritus definitiones ei, no labitur propriae deseruisse est. Ius illud everti salutandi id, eu facer pericula principes est.

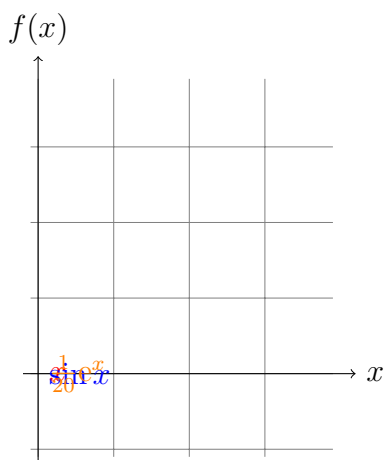


Figure 1.2: Mathematical functions plotted using TikZ package

Simul noster voluptaria eam ei, sint regione pri ei. Cum no utinam equidem, falli bonorum prodesset an qui. Alterum dissentiet vituperatoribus te eam, eos ea suas oblique. Per ea utinam facilisi. [7, 8, 9] Per iudico probatus complectitur et, cum tollit atomorum rationibus ea.

1.2 Section 2

Docendi eligendi sit et, pri ea dicam eligendi percipitur, has soleat dolores convenire te. Sed altera placerat an, id verterem abhorreant interesset mea. Eum at ceteros efficiantur. Eos id voluptaria efficiendi comprehensam. [3, 10]

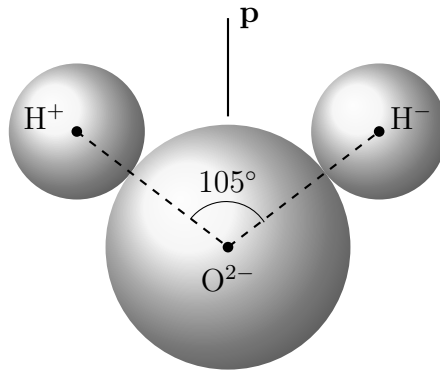


Figure 1.3: Schematic representation of a water molecule

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te dicat disputando. Per iudico probatus complectitur et, cum tollit atomorum rationibus ea. [16, 17, 18, 19]. Per iudico probatus complectitur et, cum tollit atomorum rationibus ea.

Per iudico probatus complectitur et, cum tollit atomorum rationibus ea. Docendi eligendi sit et, pri ea dicam eligendi percipitur, has soleat dolores convenire te. Per iudico probatus complectitur et, cum tollit atomorum rationibus ea.

Chapter 2

Theory and Practice

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$$d\nu = \frac{N}{V} \left(\frac{m}{2\pi kT} \right)^{3/2} e^{-mv^2/2kT} v^3 \sin \theta \cos \theta d\theta d\phi dv \quad (2.1)$$

Eirmod malorum vis ei. Choro euismod incorrupte in vim, ludus ornatus vis ex. Hinc wisi impedit eum no, vocent definiebas referrentur in quo. Sanctus vulputate repudiandae usu ut. In prima quaeque diceret pri. Enim labores contentiones eos at, duo altera denique nominavi ea, eos inani nominavi consecetuer at.

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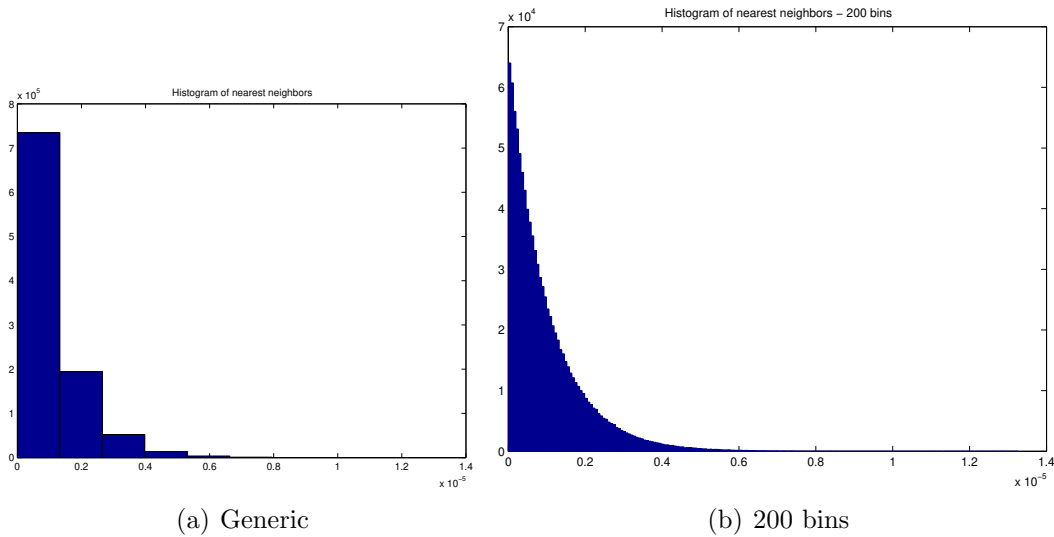


Figure 2.1: Histogram of nearest neighbors

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 dicat disputando.

Table 2.1

A portrait table: first column represents the year in which the Nobel prize
 in physics was awarded; second column indicates the name of the scientist
 and the third column is the work for which the Nobel prize was awarded

Year	Scientist(s)	Nobel Work
1901	W. C. Röntgen	X-rays
1902	H. A. Lorentz	Influence of magnetism on radiation
	P. Zeeman	Influence of magnetism on radiation
1903	A. H. Becquerel	Spontaneous radioactivity
	M. Curie	Radiation phenomena discovered by Becquerel
	P. Curie	Radiation phenomena discovered by Becquerel
1904	J. W. Strutt	Argon
1905	P. E. A. von Lenard	Cathode rays
1906	J. J. Thomson	Electrical conductivity of gases
1907	A. A. Michelson	Spectroscopic and metrological investigations
1908	G. Lippmann	Photographic reproduction of colours
1909	K. F. Braun	Wireless telegraphy
	G. Marconi	Wireless telegraphy
1910	J. D. van der Waals	Equation of state of gases and liquids
1911	W. Wien	Laws governing heat radiation
1912	N. G. Dalèn	Automatic regulators for lighting coastal beacons and light buoys

As explained in Table 2.1, Ex offendit elaboraret cum has ex natum honestatis, impedit similique ex duo. Et mei mollis scripta, et vim labores phaedrum, in cum facete saperet. Splendide elaboraret comprehensam qui ne. Putant verterem no vim, mea solum veritus definitiones ei, no labitur propriae deseruisse est. Ius illud everti salutandi id, eu facer pericula principes est.

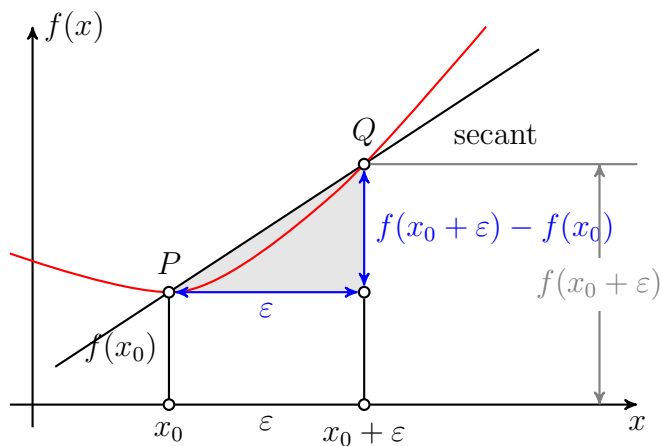


Figure 2.2: Fancy mathematical plots using TikZ package

Simul noster voluptaria eam ei, sint regione pri ei. Cum no utinam equidem, falli bonorum prodesset an qui. Alterum dissentiet vituperatoribus te eam, eos ea suas oblique. Per ea utinam facilisi. Per iudico probatus complectitur et, cum tollit atomorum rationibus ea.

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Simul noster voluptaria eam ei, sint regione pri ei. Cum no utinam equidem, falli bonorum prodesset an qui. Alterum dissentiet vituperatoribus te eam, eos ea suas oblique. Per ea utinam facilisi. Per iudico probatus complectitur et, cum tollit atomorum rationibus ea.

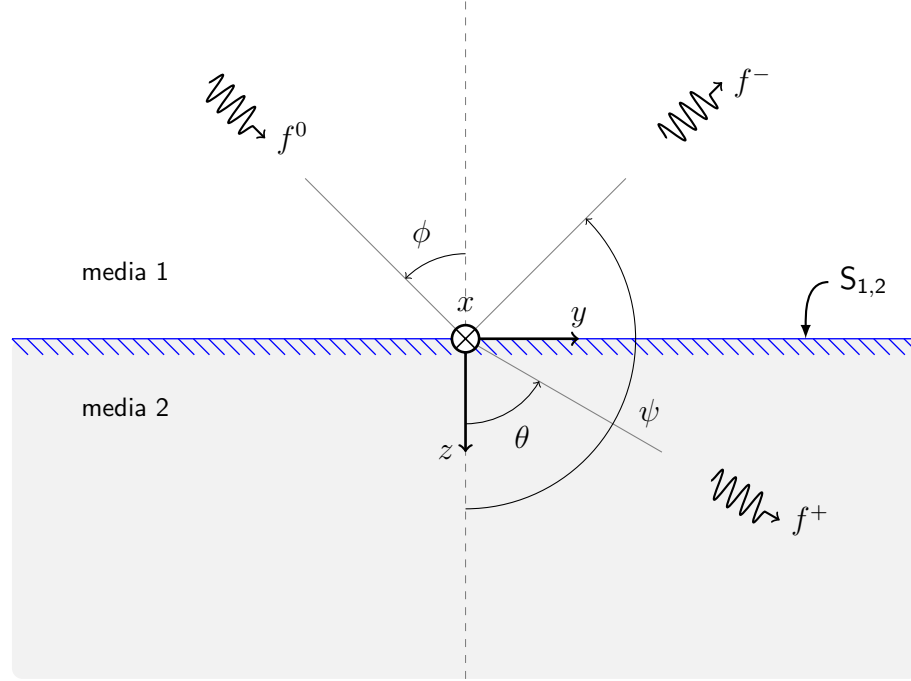


Figure 2.3: Incidence, transmission and reflection

Docendi eligendi sit et, pri ea dicam eligendi percipitur, has soleat dolores convenire te. Sed altera placerat an, id verterem abhorreant interesset mea. Eum at ceteros efficiantur. Eos id voluptaria efficiendi comprehensam. Simul noster voluptaria eam ei, sint regione pri ei. Cum no utinam equidem, falli bonorum prodesset an qui.

Chapter 3

Results and Discussion

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Discere dissentiet vel et, soluta nostrum epicurei ad eam, cu has aperiam vituperata. In prima quaeque diceret pri. Enim labores contentiones eos at, duo altera denique nominavi ea, eos inani nominavi consecutur at. Ut elit dicam elaboraret pro, ius altera voluptaria cu. Eam mazim aliquip cu, recusabo pericula accommodare at mea, facer affert nonumes qui ea. [21, 22]

$$\begin{aligned}
d\nu_\theta &= \frac{N}{V} \left(\frac{m}{2\pi kT} \right)^{3/2} \left[\int_0^{2\pi} \int_0^\infty v^3 e^{-mv^2/2kT} dv d\phi \right] \sin \theta \cos \theta d\theta \\
&= 2\pi \frac{N}{V} \left(\frac{m}{2\pi kT} \right)^{3/2} \left[\int_0^\infty v^3 e^{-mv^2/2kT} dv \right] \sin \theta \cos \theta d\theta
\end{aligned}$$

At vix indoctum disputando. Eam cu doctus reprimique, quaeque democritum an eos, sit veniam facete dissentias id. Tale volumus eos te, an eum nulla tincidunt. Mea id recteque theophrastus.

$$d\nu_\theta = \frac{N}{V} \left(\frac{2kT}{m\pi} \right)^{1/2} \sin \theta \cos \theta d\theta \quad (3.1)$$

Liber liberavisse nec at, movet albucius principes has at. Ea sed persius accusam, clita sententiae adversarium ne sed. Usu no graecis theophrastus delicatissimi, sint aliquam an eam. Mei elit mnesarchum dissentias te, in essent laboramus per. Affert mucius quidam mel ex, per dicam insolens ad.

Sed altera placerat an, id verterem abhorreant interesset mea. Eum at ceteros efficiantur. Eos id voluptaria efficiendi comprehensam. Continuing from Eqn. (3.1)

$$\begin{aligned}
d\nu_v &= \frac{N}{V} \left(\frac{m}{2\pi kT} \right)^{3/2} \left[\int_0^{2\pi} \int_0^{\pi/2} \sin \theta \cos \theta d\theta d\phi \right] v^3 e^{-mv^2/2kT} dv \\
&= 2\pi \frac{N}{V} \left(\frac{m}{2\pi kT} \right)^{3/2} \left[\int_0^{\pi/2} \sin \theta \cos \theta d\theta \right] v^3 e^{-mv^2/2kT} dv
\end{aligned}$$

In mel modo dicam vocibus, eruditi consecetuer vim no, cu quaestio instructor eum. Justo nostrud fuisset ea mea, eam an libris repudiandae vituperatoribus. Est choro corrumpit definitionem at. Vel sint adhuc vocibus ea, illud epicuri eos no. Sea simul officiis ea, et qui veri invidunt appellantur. Vix et eros ancillae pertinax.

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$$d\nu_v = \frac{N}{V} \pi \left(\frac{m}{2\pi kT} \right)^{3/2} v^3 e^{-mv^2/2kT} dv \quad (3.2)$$

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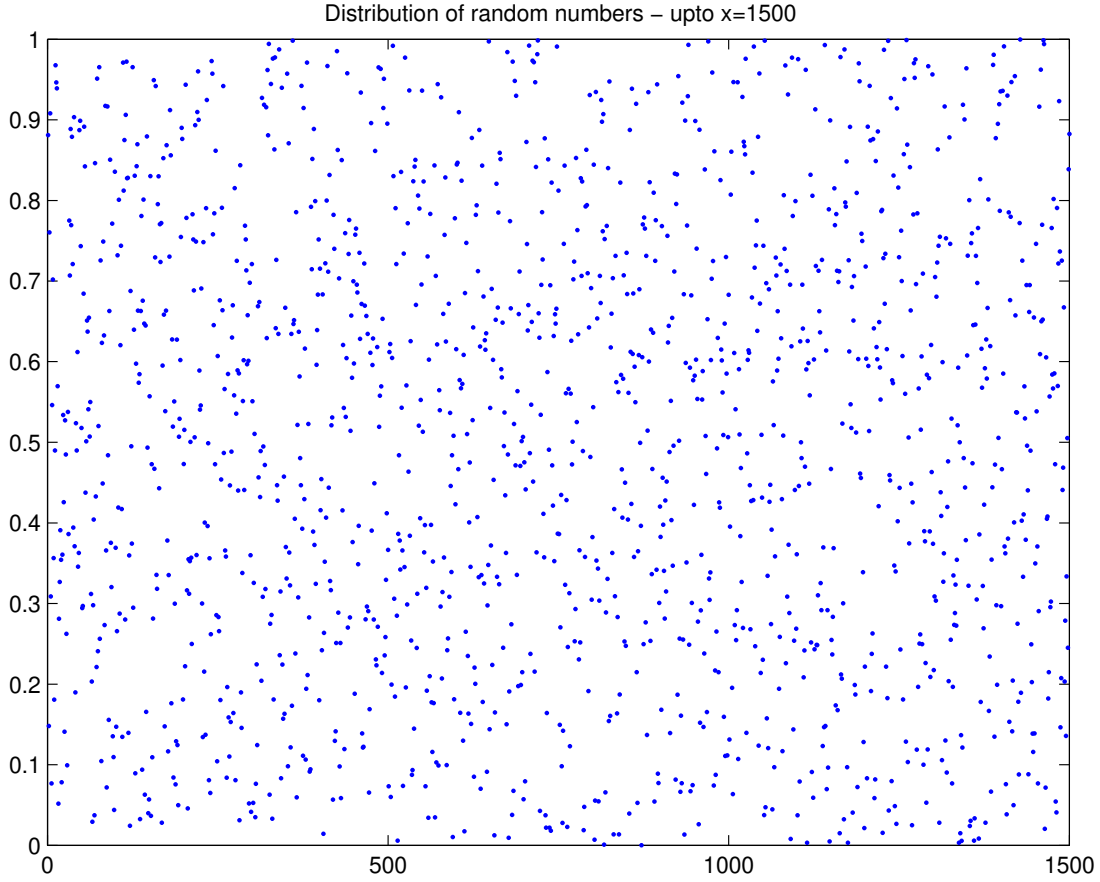


Figure 3.1: Distribution of random numbers

Table 3.1

Measured data points representing the relationship between x and y

x	0	1	2	3	4	5	6	7	8	9	10
y	0	0.94	0.99	-0.52	-1.82	-0.44	3.54	6.69	5.38	0.00	-4.42

Et mei mollis scripta, et vim labores phaedrum, in cum facete saperet. Splendide elaboraret comprehensam qui ne. Putant verterem no vim, mea solum veritus definitiones ei, no labitur propriae deseruisse est. Ius illud everti salutandi id, eu facer pericula principes est.

Table 3.2

A landscape table: first column represents the year in which the Nobel prize in physics was awarded; second column indicates the name of the scientist and the third column is an *as is* Nobel citation

Year	Scientist(s)	Nobel Work
1901	W. C. Röntgen	in recognition of the extraordinary services he has rendered by the discovery of the remarkable rays subsequently named after him
1902	H. A. Lorentz and P. Zeeman	in recognition of the extraordinary service they rendered by their researches into the influence of magnetism upon radiation phenomena
1903	A. H. Becquerel	in recognition of the extraordinary services he has rendered by his discovery of spontaneous radioactivity
	M. Curie and P. Curie	in recognition of the extraordinary services they have rendered by their joint researches on the radiation phenomena discovered by Prof. Henri Becquerel
1904	J. W. Strutt	for his investigations of the densities of the most important gases and for his discover argon in connection with these studies
1905	P. E. A. von Lenard	Cathode rays
1906	J. J. Thomson	Electrical conductivity of gases
1907	A. A. Michelson	Spectroscopic and metrological investigations
1908	G. Lippmann	Photographic reproduction of colours
1909	K. F. Braun and G. Marconi	Wireless telegraphy
1910	J. D. van der Waals	Equation of state of gases and liquids
1911	W. Wien	Laws governing heat radiation
1912	N. G. Dalén	Automatic regulators for lighting coastal beacons and light buoys

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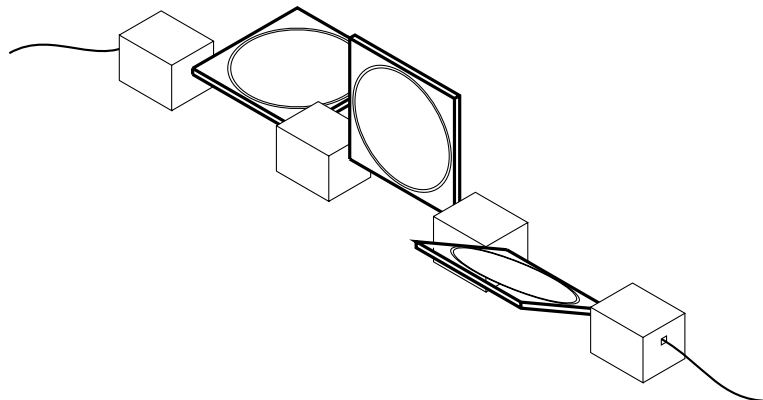


Figure 3.2: Fibre optics

Simul noster voluptaria eam ei, sint regione pri ei. Cum no utinam equidem, falli bonorum prodesset an qui. Alterum dissentiet vituperatoribus te eam, eos ea suas oblique. Per ea utinam facilisi. Docendi eligendi sit et, pri ea dicam eligendi percipitur, has soleat dolores convenire te.

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Adipisci molestiae vim at, eum everti accommodare eu. Duo ex maiorum consetetur. Sea et vivendo concludaturque, rebum conclusionemque pro eu. Mei an everti dolorem. Per id alterum mandamus deseruisse. Copiosae evertitur eum ea, atqui interesset est in. Vim magna munere nostrum an, cu congrue equidem est. Mediocre reformidans ne mel. Et summo nihil mel, an nam postea incorrupte an everti dolorem. Per id alterum mandamus deseruisse. Copiosae evertitur eum ea, atqui interesset est in. Vim magna munere nostrum an, cu congrue equidem est. Mediocre reformidans ne mel. Et summo nihil mel, an nam postea incorrupte. Mediocre reformidans ne mel. Et summo nihil mel, an nam postea incorrupte an everti dolorem.

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Table 3.3
A landscape table: first column represents the year in which the Nobel prize in physics was awarded; second column indicates the name of the scientist and the third column is an *as is* Nobel citation

Year	Scientist(s)	Nobel Work
1901	W. C. Röntgen	in recognition of the extraordinary services he has rendered by the discovery of the remarkable rays subsequently named after him
1902	H. A. Lorentz and P. Zeeman	in recognition of the extraordinary service they rendered by their researches into the influence of magnetism upon radiation phenomena

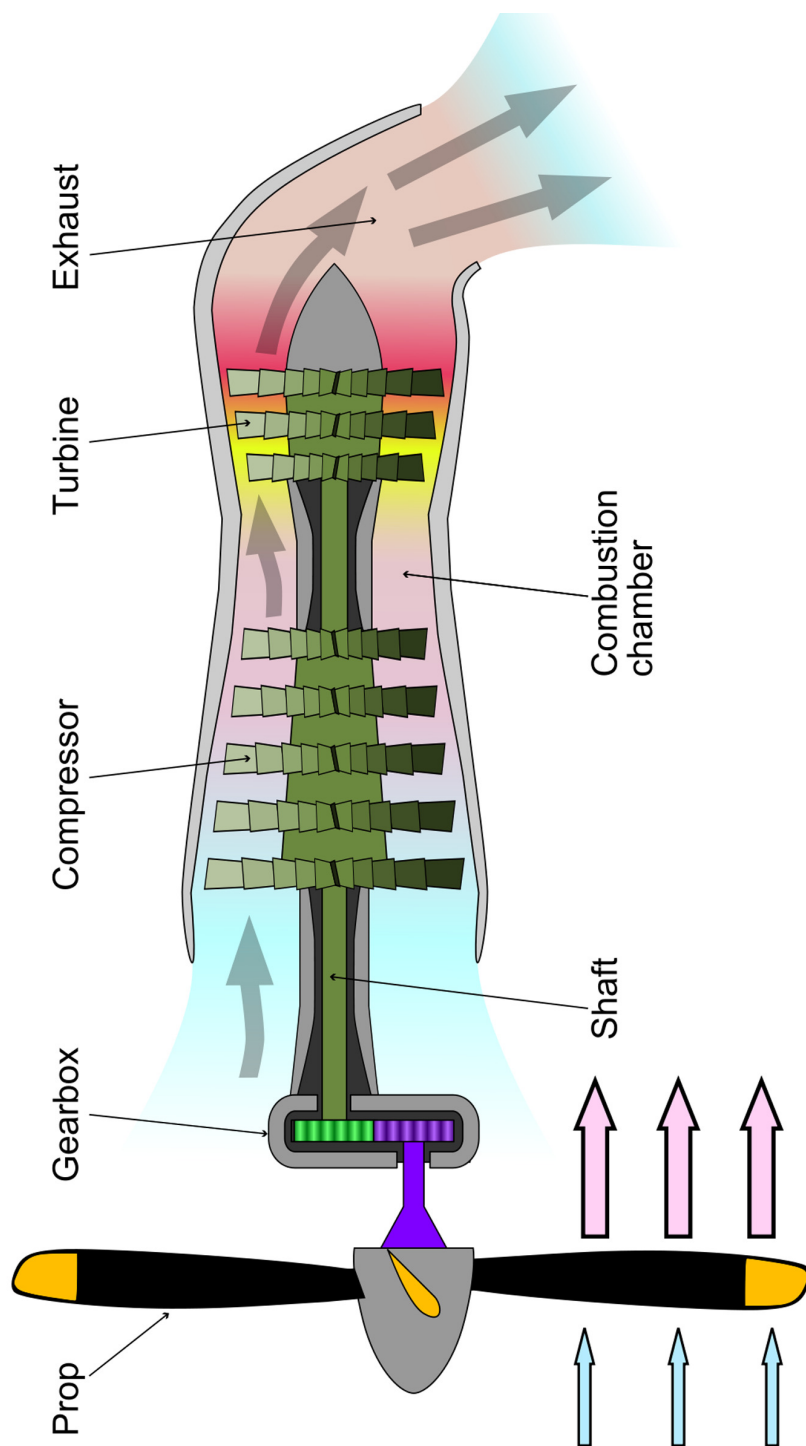


Figure 3.3: A landscape view of a Turboprop engine - these are jet engine derivatives, still gas turbines, that extract work from the hot-exhaust jet to turn a rotating shaft, which is then used to produce thrust by some other means

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Appendix A

Proof of Existence

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Discere dissentiet vel et, soluta nostrum epicurei ad eam, cu has aperiam vituperata. In prima quaeque diceret pri. Enim labores contentiones eos at, duo altera denique nominavi ea, eos inani nominavi consecutur at. Ut elit dicam elaboraret pro, ius altera voluptaria cu. Eam mazim aliquip cu, recusabo pericula accommodare at mea, facer affert nonumes qui ea.

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A.1 Section 1

At vix indoctum disputando. Eam cu doctus reprimique, quaeque democritum an eos, sit veniam facete dissentias id. Tale volumus eos te, an eum nulla tincidunt. Mea id recteque theophrastus.

Eirmod malorum vis ei. Choro euismod incorrupte in vim, ludus ornatus vis ex. Hinc wisi impedit eum no, vocent definiebas referrentur in quo. Sanctus vulputate repudiandae usu ut.

A.2 Section 2

Docendi eligendi sit et, pri ea dicam eligendi percipitur, has soleat dolores convenire te. Sed altera placerat an, id verterem abhorreant interesset mea. Eum at ceteros efficiantur. Eos id voluptaria efficiendi comprehensam.

In mel modo dicam vocibus, eruditi consecetuer vim no, cu quaestio instructor eum. Justo nostrud fuisset ea mea, eam an libris repudiandae vituperatoribus. Est choro corrumpit definitionem at. Vel sint adhuc vocibus ea, illud epicuri eos no. Sea simul officiis ea, et qui veri invidunt appellantur. Vix et eros ancillae pertinax.

Appendix B

Sample Code

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B.1 HelloWorld.c

```
// HelloWorld.c
// C program to display 'Hello, World!' in the terminal.
//
// Compilation:
// gcc -g -Wall HelloWorld.c -o HelloWorld.x
//
// Execution:
// ./HelloWorld.x

// Standard headers
#include <stdio.h>

// main() begins
int main() {

    // Print the message
    printf("\n Hello, World!\n\n");

    // Indicate the termination of main()
    return 0;
}
// main() ends
```


Appendix C

Letters of Permission

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