

EI MEL QUAS NULLAM CONSTITUTO, NAM TE TIMEAM MENTITUM

By

John D. Sanderson

A DISSERTATION

Submitted in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

In SOME-PROGRAM

MICHIGAN TECHNOLOGICAL UNIVERSITY

2014

© 2014 John D. Sanderson

This dissertation has been approved in partial fulfillment of the requirements for the Degree of DOCTOR OF PHILOSOPHY in SOME-PROGRAM.

PROGRAM: SOME-PROGRAM

Dissertation Co-advisor: Dr. Co-advisor #1

Dissertation Co-advisor: Dr. Co-advisor #2

Committee Member: Dr. Advisory Committee #1

Committee Member: Dr. Advisory Committee #2

Committee Member: Dr. Advisory Committee #3

Committee Member: Dr. Advisory Committee #4

School Dean: Dr. School Dean

Dedication

To my mother, teachers and friends

who didn't hesitate to criticize my work at every stage - without which I would neither
be who I am nor would this work be what it is today.

Contents

List of Figures	ix
List of Tables	xi
Preface	xiii
Acknowledgments	xv
Abstract	xvii
1 Introduction	1
1.1 Section 1	2
1.1.1 Subsection 1	2
1.1.2 Subsection 2	3
1.2 Section 2	4
2 Theory and Practice	5
3 Results and Discussion	9
References	17

A	Proof of Existence	21
A.1	Section 1	22
A.2	Section 2	22
B	Sample Code	23
B.1	HelloWorld.c	24
C	Letters of Permission	25

List of Figures

2.1	Histogram of nearest neighbors	6
	(a) Generic	6
	(b) 200 bins	6
3.1	Distribution of random numbers	12
3.2	A landscape view of a Turboprop engine - these are jet engine deriva- tives, 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	15

List of Tables

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	7
3.1	Measured data points representing the relationship between x and y	12
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 <i>as is</i> Nobel citation	13

Preface

Lorem ipsum dolor sit amet, consectetur adipisicing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

Sed ut perspiciatis unde omnis iste natus error sit voluptatem accusantium doloremque laudantium, totam rem aperiam, eaque ipsa quae ab illo inventore veritatis et quasi architecto beatae vitae dicta sunt explicabo. Nemo enim ipsam voluptatem quia voluptas sit aspernatur aut odit aut fugit, sed quia consequuntur magni dolores eos qui ratione voluptatem sequi nesciunt.

Lorem ipsum dolor sit amet, consectetur adipisicing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

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 \LaTeX .

Lorem ipsum dolor sit amet, consectetur adipisicing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

Neque porro quisquam est, qui dolorem ipsum quia dolor sit amet, consectetur, adipisci velit, sed quia non numquam eius modi tempora incidunt ut labore et dolore magnam aliquam quaerat voluptatem. Ut enim ad minima veniam, quis nostrum exercitationem ullam corporis suscipit laboriosam, nisi ut aliquid ex ea commodi consequatur? Quis autem vel eum iure reprehenderit qui in ea voluptate velit esse quam nihil molestiae consequatur, vel illum qui dolorem eum fugiat quo voluptas nulla pariatur?

Abstract

This provides information on how to write your MS thesis or PhD dissertation using the \LaTeX document preparation system in compliance with Michigan Technological University Graduate School requirements.

Lorem ipsum dolor sit amet, consectetur adipisicing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

Sed ut perspiciatis unde omnis iste natus error sit voluptatem accusantium doloremque laudantium, totam rem aperiam, eaque ipsa quae ab illo inventore veritatis et quasi architecto beatae vitae dicta sunt explicabo. Nemo enim ipsam voluptatem quia voluptas sit aspernatur aut odit aut fugit, sed quia consequuntur magni dolores eos qui ratione voluptatem sequi nesciunt.

Chapter 1

Introduction

Lorem ipsum dolor sit amet, at qui viderer recusabo aliquando, dignissim evertitur ei his. Ignota iuvaret fabulas ei vim. Ne utinam inciderint quo. Pri ea congrue postulant conclusionemque. Ut elit dicam elaboraret pro, ius altera voluptaria cu. Eam mazim aliquip cu, recusabo pericula accommodare at mea, facer affert nonumes qui ea.

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]

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]

Aliquip lobortis ei est, at error viris graeco sed. Vel te elitr detracto, modo graecis scripserit ex nec. Errem utamur viderer per no, eam ea eripuit referrentur. Pro te dicat disputando.

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.

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]

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. [11, 12, 13, 14, 15] Per iudico probatus complectitur et, cum tollit atomorum rationibus ea. Per iudico probatus complectitur et, cum tollit atomorum rationibus ea.

Aliquip lobortis ei est, at error viris graeco sed. Vel te elitr detracto, modo graecis scripserit ex nec. Errem utamur viderer per no, eam ea eripuit referrentur. Pro 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

Lorem ipsum dolor sit amet, at qui viderer recusabo aliquando, dignissim evertitur ei his. Ignota iuvaret fabulas ei vim. Ne utinam inciderint quo. Pri ea congrue postulant conclusionemque. [20] Discere dissentiet vel et, soluta nostrum epicurei ad eam, cu has aperiam vituperata.

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.

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

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.

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.



Figure 2.1: Histogram of nearest neighbors

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.

Aliquip lobortis ei est, at error viris graeco sed. Vel te elitr detracto, modo graecis
 scripserit ex nec. Errem utamur viderer per no, eam ea eripuit referrentur. Pro te
 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.

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.

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.

Chapter 3

Results and Discussion

Lorem ipsum dolor sit amet, at qui viderer recusabo aliquando, dignissim evertitur ei his. Ignota iuvaret fabulas ei vim. Ne utinam inciderint quo. Pri ea congrue postulant conclusionemque. In prima quaeque diceret pri. Enim labores contentiones eos at, duo altera denique nominavi ea, eos inani nominavi consecetur at. Ut elit dicam elaboraret pro, ius altera voluptaria cu.

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 consecetur 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.

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.

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

Aliquip lobortis ei est, at error viris graeco sed. Vel te elitr detracto, modo graecis scripserit ex nec. Errem utamur viderer per no, eam ea eripuit referrentur. Pro te dicat disputando.



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. Dalèn	Automatic regulators for lighting coastal beacons and light buoys

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.

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.

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.

In amet verear evertitur qui, ex mea vivendo hendrerit. Ad posse perfecto prodesset usu, cum fugit accumsan no. Tempor nonumes duo ea, oblique fabulas salutatus ne vis. Ne eam scripta dolorem, graece eruditi eum ei. Ei sed brute zril nostro, nostro voluptatum id sea, courtesy of Wikipedia. [23] Adipisci molestiae vim at, eum everti accommodare eu. Duo ex maiorum consetetur. Sea et vivendo concludaturque, rebum conclusionemque pro eu.



Figure 3.2: 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

Id ius soluta semper audiam, ad eos scriptorem concludaturque, id mel rebum volumus deserunt. Mel libris percipit scriptorem te, his an dicat putent menandri, mazim officiis aliquando mei no. Ne clita veniam disputando vim, postea hendrerit maiestatis qui id. Mei te suscipit quaerendum, an aliquando intellegebat ius, ei simul detraxit dissentiet eam. Zril dolor ut usu.

Everti saperet vis ut. Scripta maluisset mel eu, duis antiopam in pro. Sea diceret contentiones ea. Nec eu duis efficiantur, evertitur constituam mediocritatem te vis, pro error regione ad. Sit malorum aliquam at, pericula dissentias mei ei. Cu soluta urbanitas est, albucius vituperatoribus usu et.

References

- [1] Dovesi, R.; Orlando, R.; Civalleri, B.; Roetti, C.; Saunders, V. R.; Zicovich-Wilson, C. M. *Zeitschrift für Kristallographie* **2005**, *220*, 571.
- [2] Delley, B. *Journal of Chemical Physics* **1990**, *92*, 508.
- [3] Dongarra, J. J.; Croz, J. D.; Hammarling, S.; Duff, I. S. *Association for Computing Machinery Transactions on Mathematical Software* **1990**, *16*, 1.
- [4] Car, R.; Parrinello, M. *Physical Review Letters* **1985**, *55*, 2471.
- [5] CPMD (v3.15.1): An *ab initio* Electronic Structure and Molecular Dynamics Program. The CPMD Consortium, **2011**.
- [6] Crystal 09 user's manual. Dovesi, R.; Saunders, V. R.; Roetti, C.; Orlando, R.; Zicovich-Wilson, C. M.; Pascale, F.; Civalleri, B.; Doll, K.; Harrison, N. M.; Bush, I. J.; D'Arco, P.; Llunell, M.; University of Torino, Italy, **2009**.
- [7] Dongarra, J. J.; Bunch, J.; Moler, C.; Stewart, G. W. *LINPACK User's Guide*; Society for Industrial and Applied Mathematics, Philadelphia, PA, 1979.

- [8] Delley, B. *Journal of Physical Chemistry* **1996**, *100*, 6107.
- [9] Dongarra, J. J. *Argonne National Laboratory Report, ANL-80-24* **1980**.
- [10] Dongarra, J. J.; Croz, J. D.; Hammarling, S.; Hanson, R. *Association for Computing Machinery Transactions on Mathematical Software* **1988**, *14*, 1.
- [11] Hess, B.; Kutzner, C.; van der Spoel, D.; Lindahl, E. *Journal of Chemical Theory and Computation* **2008**, *4*, 235.
- [12] Gale, J. D. *Journal of Chemical Society, Faraday Transactions* **1997**, *93*, 629.
- [13] Gale, J. D. *Philosophical Magazine B* **1996**, *73*, 3.
- [14] Falgout, R. D.; Yang, U. M. In *Proceedings of the International Conference on Computational Science - Part III, ICCS '02*, page 632, London, UK, 2002. Springer-Verlag.
- [15] Plimpton, S. J. *Journal of Computational Physics* **1995**, *117*, 1.
- [16] R: A Language and Environment for Statistical Computing. R Development Core Team.; R Foundation for Statistical Computing, Vienna, Austria, **2011**.
- [17] Soler, J. M.; Artacho, E.; Gale, J. D.; García, A.; Junquera, J.; Ordejón, P.; Sánchez-Portal, D. *Journal of Physics: Condensed Matter* **2002**, *14*, 2745.
- [18] Ordejón, P.; Drabold, D. A.; Grumbach, M. P.; Martin, R. M. *Physical Review B* **1993**, *48*, 14646.

- [19] Rungger, I.; Sanvito, S. *Physical Review B* **2008**, *78*, 035407.
- [20] Rocha, A. R. *Theoretical and Computational Aspects of Electronic Transport at the Nanoscale* PhD thesis, University of Dublin, Trinity College, **2007**.
- [21] Anderson, E.; Bai, Z.; Bischof, C.; Blackford, S.; Demmel, J.; Dongarra, J. J.; Croz, J. D.; Greenbaum, A.; Hammarling, S.; McKenney, A.; Sorensen, D. *LA-PAACK Users' Guide*; Society for Industrial and Applied Mathematics: Philadelphia, PA, 3 ed., 1999.
- [22] Frigo, M.; Johnson, S. G. In *Proceedings of the IEEE*, Vol. 93, page 216, 2005.
- [23] <http://wikipedia.org/>. *Wikipedia*; Wikipedia: The Internet, 2012.
- [24] Kresse, G.; Hafner, J. *Physical Review B* **1993**, *47*, 558.
- [25] Kresse, G.; Hafner, J. *Physical Review B* **1994**, *49*, 14251.
- [26] Schaftenaar, G.; Noordik, J. H. *Journal of Computer-Aided Molecular Design* **2000**, *14*, 123.
- [27] Humphrey, W.; Dalke, A.; Schulten, K. *Journal of Molecular Graphics* **1996**, *14*, 33.
- [28] Kolkaji, A. *Molecular Graphics Modelling* **1999**, *17*, 176.

Appendix A

Proof of Existence

Lorem ipsum dolor sit amet, at qui viderer recusabo aliquando, dignissim evertitur ei his. Ignota iuvaret fabulas ei vim. Ne utinam inciderint quo. Pri ea congrue postulant conclusionemque.

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.

Lorem ipsum dolor sit amet, at qui viderer recusabo aliquando, dignissim evertitur ei his. Ignota iuvaret fabulas ei vim in Section A.1.

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

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.

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.

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.

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

Include letters of permission from journal editors and/or other sources from which you may have used materials (images, information, etc.) in this this work.

These materials may also be submitted separately to the Graduate School as a single, well-organized PDF file.