UF ETD $\LaTeX\,2_\varepsilon$ THESIS AND DISSERTATION TEMPLATE TUTORIAL

By

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A TUTORIAL PRESENTED TO THE GRADUATE SCHOOL
OF THE UNIVERSITY OF FLORIDA IN PARTIAL FULFILLMENT
OF THE REQUIREMENTS FOR THE DEGREE OF
MASTER OF THE UNIVERSE

UNIVERSITY OF FLORIDA

2016

I dedicate this to everyone that helped revamp this template. Aliquam molestie sed urna quis convallis. Aenean nibh eros, aliquam non eros in, tempus lacinia justo. In magna sapien, blandit a faucibus ac, scelerisque nec purus. Praesent fermentum felis nec massa interdum, vel dapibus mi luctus. Cras id fringilla mauris. Ut molestie eros mi, ut hendrerit nulla tempor et. Pellentesque tortor quam, mattis a scelerisque nec, euismod et odio. Mauris rhoncus metus sit amet risus mattis, eu mattis sem interdum.

ACKNOWLEDGMENTS

Thanks to all the help I have received in writing and learning about this tutorial. Acknowledgments are required and must be written in paragraph form. This mandates at least three sentences.

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of the University of Florida in Partial Fulfillment of the
Requirements for the Degree of Master of the Universe

UF ETD LaTeX 2_εTHESIS AND DISSERTATION TEMPLATE TUTORIAL

By

James Booth

May 2016

Chair: James B. Albury
Major: Electronic Thesis and Dissertations

Abstracts should be less than 350 words. Any Greek letters or symbols not found on a standard computer keyboard will have to be spelled out in the electronic version so try to avoid them in the Abstract if possible. The best way to compile the document is to use the make_xelatex.bat file. If you are using Linux or Macintosh Operating Systems there are examples of make files for these systems in the Make Files Folder but they may be outdated and need to be modified for them to work properly. This document is the official tutorial outlining the use and implementation of the UF LaTeX2ϵ Template for use on thesis and dissertations. The tutorial will cover the basic files, commands, and syntax in order to properly implement the template. It should be made clear that this tutorial will not tell one how to use LaTeX2ϵ. It will be assumed that you will have had some previous knowledge or experience with LaTeX2ϵ, but, there are many aspects of publishing for the UF Graduate School that requires attention to some details that are normally not required in LaTeX2ϵ.

Pay particular attention to the section on references. NONE of the bibliography style files (.bst) are an assurance that your document's reference style will meet the Editorial Guidelines. You MUST get a .bst file that matches the style used by the journal you used as a guide for your references and citations. The files included in this document are examples only and are NOT to be used unless they match your sample article exactly!

You should have a .bib file (we have included several examples) that contains your reference sources. Place your .bib file in the bib folder and enter the name of the file in the list of bib files, or enter your reference information into one of our existing .bib files if you don't already have one. Just make sure to preserve the format of each kind of reference. Each time you cite a reference you enter the ”key” (the first field in the reference listing in the .bib file) associated with that reference. During the compilation process LaTeX will gather all the references, insert the correct method of citation and list the references in the correct location in the proper format for the reference style selected.

CHAPTER 1
INTRODUCTION AND OPENING REMARKS

We don't make the Chapter titles in All Caps Automatically because it is easier for you to type your Chapter Titles in uppercase than for those that need to have mixed case in their titles to find the correct command in the ufthesis.cls file and change it there. [*] We don't recommend that you change much of anything in the class file unless you're absolutely sure of what your are doing.[1]

1.1 The Section Command Text Should Be in Title Case

Title case is where all principal words are capitalized except prepositions, articles, and conjunctions. [1]

1.1.1 Subsection Commands Are Also in Title Case

The difference, of course, are the second level headings are left-aligned

1.1.1.1 Subsubsections are in sentence case

The third level subheadings are left-aligned but in sentence case. Only the first letter and any proper nouns are capitalized. [2]

1.1.1.2 If you divide a section, you must divide it into two, or more, parts

Paragraph headings. There is no official fourth level heading. Do not use the Paragraph heading feature in LaTeX, simply apply the bold characteristic to the first few words of a paragraph followed by a colon or period.

1.1.2 I Need Another Second Level Heading in This Section

Aliquam mi nisi, tristique at rhoncus quis, consectetur non mi. Phasellus blandit quam ligula, a viverra lacus commodo at. In iaculis nisl vel pretium sollicitudin. In

[*] an un-numbered footnote - this is how you tell the readers that this chapter was previously published and then cite the Journal where it was published

[1] and now we're back to normal footnote marking

efficitur massa vel elit sollicitudin, vel auctor sapien cursus. Proin feugiat sapien a mi tempus;

$X - X' = D + D'$

in consequat augue cursus. Nulla sed sagittis purus. Nunc eu consequat orci, eu laoreet enim. Ut euismod tincidunt sem, eget lacinia dui luctus eu. Aliquam mi augue, faucibus id semper vitae, porta ac ligula. Morbi sed ultrices odio. Mauris id luctus ex. Nulla ac libero dictum, interdum turpis lacinia, scelerisque leo. Praesent varius orci ac eros varius pharetra.

1.2 Image Handling in XeLaTeX

One of the biggest reasons for switching from the dvipdfm/dvipdfmx methods of compiling is the improved image handling capabilities. EPS, Bit-mapped, PDF, JPG, and PNG formats work well with the xelatex process.

1.2.1 The Traditional EPS Format

EPS format is the traditional format for LaTeX, but EPS files can be very large and many programs can't create or view these images. There are many programs that are used to interpret data and output the results as an EPS format image. It has been my experience that there are bounding box problems with these figures. On many occasions we have opened the image in Adobe Photoshop and, without making any changes, saved the document as a Photoshop EPS file, re-compiled the document, and the image worked correctly, so if you are having problems with an EPS image not showing in your document correctly, try this fix first.

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1.2.2 Bitmapped Images Work As Well

Bitmapped images are a standard file type on PCs, but these files are also usually very large so compressed images may be a better alternative.

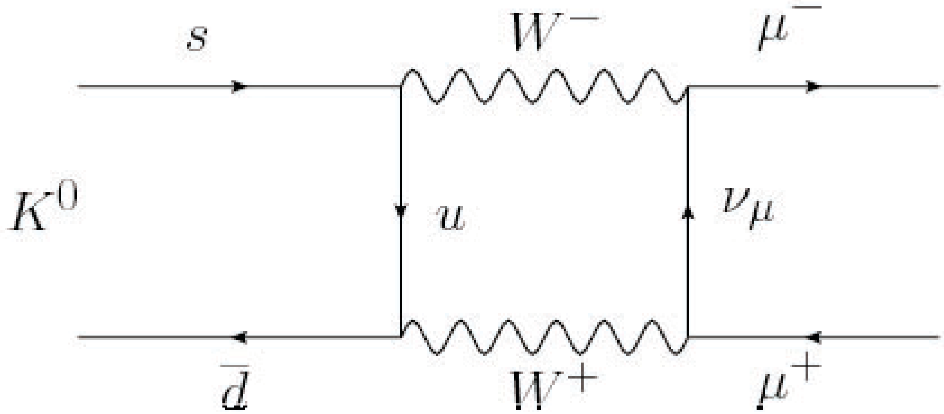

Figure 1-1. EPS format diagram. Note: no filetype is designated by adding an extension. The file type is determined and the correct procedure is automatically chosen by xelatex.

Figure 1-2. BMP format drawing. Note: no filetype is designated by adding an extension. The file type is determined and the correct procedure is automatically chosen by xelatex.

Morbi hendrerit risus nec quam posuere viverra. Donec quis tellus faucibus, molestie arcu sed, congue urna. Duis eget neque ac libero pulvinar porta eget et magna. Donec a magna eu eros suscipit cursus ac vitae nisl. Vivamus ligula purus, congue sed tortor blandit, ultrices egestas nisl.

1.2.3 Not to Mention PDF

It is often very handy to be able to include a pdf file as an image. By using XeLaTeX this is usually just matter of setting the size, or scale properties correctly.

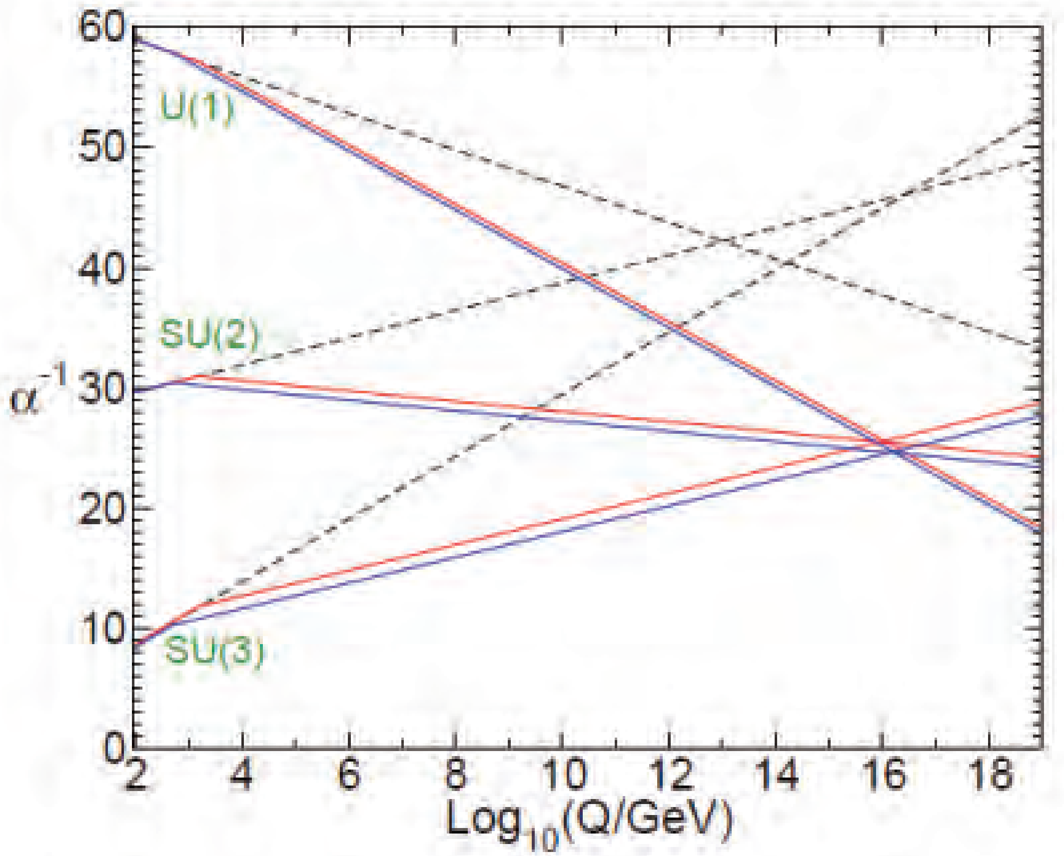

Figure 1-3. PDF format graph. Note: no filetype is designated by adding an extension. The file type is determined and the correct procedure is automatically chosen by xelatex.

Nulla mattis augue lacus. Nam non lectus dolor. Cras ac quam vel justo elementum vestibulum. Integer vulputate pulvinar lacus sit amet pulvinar.

1.2.4 JPG Is Absolutely Necessary

For photographs, JPG is the most common format. This format is a fraction of the size of Bit-mapped images and can deliver very good quality at a much smaller overhead. Vestibulum eu lectus vel orci dictum vehicula. Proin id maximus dolor. Integer augue ante, pulvinar ac erat vitae, porttitor ullamcorper libero. [3]

Figure 1-4. JPG format image. Note: no filetype is designated by adding an extension. The file type is determined and the correct procedure is automatically chosen by xelatex.

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1.2.5 PNGs Will Help Make Files Smaller

PNG files are even smaller than JPGs and are very good when text and images are combined.

Figure 1-5. PNG format map. Note: no filetype is designated by adding an extension. The file type is determined and the correct procedure is automatically chosen by xelatex.

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1.3 GIF, TIF, and Others

Other file formats have not been successful, with or without file extensions. The tests have not been exhaustive so if you have a different type, give it a try. GIF, and TIF both do NOT work at this time. The next image demonstrates how to use multiple images as a single figure. Notice, there is a single caption for ALL figures and that caption starts with a discription of the ENTIRE figure before breaking off into the subfigure descriptions.

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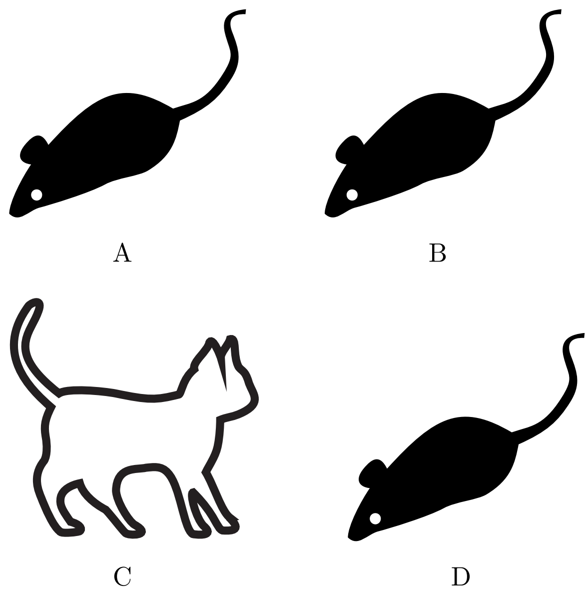

Figure 1-6. Tom and Jerries. This caption demonstrates how the sub-captions are left out of the List of Figures, but included in the figure itself. A) Tom the first; B) Tom the second; C) Jerry; D) Tom the third.

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Nunc blandit scelerisque velit, ac facilisis dui finibus et. Sed facilisis tortor vel commodo luctus. Donec est felis, malesuada id nibh in, accumsan malesuada lectus.

- WinEDT: This text editor is recommended for use editing TEX-files as it has many useful built in macros and is easy to use
- This program can be found and downloaded here: http://www.winedt.com/
- The GIMP (GNU Image Manipulation Program)
  - A freeware graphics editing program for picture editing and file conversions
  - Comparable to Adobe Photoshop
  - Can be downloaded here: http://www.gimp.org/
- A good reference of LATEX2ϵ commands

– This should be included on the ETD website here: http://etd.helpdesk.ufl.edu/tex.php

Sed lobortis volutpat felis, vitae aliquet augue congue id. Fusce ut odio tincidunt, condimentum nulla vel, pharetra arcu. In ultricies libero diam, nec rutrum magna vehicula nec. Praesent dictum eros sit amet turpis ultricies, eleifend condimentum dui imperdiet. Donec congue urna ante, id rutrum mi commodo a. Vivamus id tincidunt nunc. Morbi id lacus ut augue ultricies convallis. Duis a lectus quis ante pretium scelerisque nec nec nisi. In id porta justo, at euismod diam. Suspendisse vel tempus arcu. Praesent vel cursus nisi, ac rhoncus odio.

CHAPTER 2
GENERALIZED SCALAR APPROACH TO EMPIRICAL POTENTIAL PARAMETERIZATION

This chapter reviews typical approaches to fitting empirical potentials.

2.1 Theoretical Background on Potentials

The justification for the use of classical empirical potentials can be demonstrated from the Born-Oppenheimer approximation[**?**]. The Hamiltonian for a real material is defined by the presence of interacting nuclei and electrons:

$$H = \sum_i \frac{P_i}{2M_i} + \sum_\alpha \frac{p_\alpha}{2m} + \frac{1}{2}\sum_{ij} \frac{Z_i Z_j e^2}{r_{ij}} + \frac{1}{2}\sum_{\alpha\beta} \frac{e^2}{r_{\alpha\beta}} - \sum_{i\alpha} \frac{Z_i e^2}{r_{i\alpha}} \tag{2–1}$$

The first terms are kinetic energy terms, the latter terms are the nuclei-nuclei, electron-electron, and nuclei-electron interactions. Ideally, the solution of Schrödinger's equation, $H\Psi = E\Psi$ could be solved providing the total wavefunction $\Psi(\boldsymbol{r}_i, \boldsymbol{r_\alpha})$. Except for the simplest of systems, this approach is impossible computationally. The Born-Oppenheimer approximation [**?**] is ubiquitous in *ab initio* calculations, and forms the justification for classical empirical potentials. The kinetic energy is ignored since the heavy nulclei move more slowly than electrons. For the remaining interaction terms of the Hamiltonian, the nuclear positions are clamped at certain positions in space, the electron-nuclei interactions are not removed, since the electrons are still influenced by the Coulomb potential of the nuclei. This allows us to factor the wavefunction as

$$\Psi(\boldsymbol{R}_i, \boldsymbol{r}_\alpha) = \Xi(\boldsymbol{R}_i)\Phi(\boldsymbol{r}_\alpha; \boldsymbol{R}_i) \tag{2–2}$$

, where $\Xi(\boldsymbol{R}_i)$ describes the nuclei, and $\Phi(\boldsymbol{r}_\alpha; \boldsymbol{R}_i)$ describes the electrons parameterized by the clamped position of $\boldsymbol{R}_i$. In turn, the Hamiltonian is solve able as two Schrödinger's equations. The first equation contains the electronic degrees of freedom.

$$H_e\Phi(\boldsymbol{r}_\alpha; \boldsymbol{R}_i) = U(\boldsymbol{R}_i)\Phi(\boldsymbol{r}_\alpha; \boldsymbol{R}_i) \tag{2–3}$$

where

$$H_e = \sum_{\alpha} \frac{p_\alpha}{2m} + \frac{1}{2}\sum_{ij} \frac{Z_i Z_j e^2}{r_{ij}} + \frac{1}{2}\sum_{\alpha\beta} \frac{e^2}{r_{\alpha\beta}} - \sum_{i\alpha} \frac{Z_i e^2}{r_{i\alpha}} \tag{2–4}$$

Eqn. 2–3 gives the energy $U(\boldsymbol{R}_i)$ which depends on the clamped coodinates of $\boldsymbol{R}_i$. The electronic effects are contained in $U(\boldsymbol{R}_i)$ and is incorporated into the second equation which the motion of the nuclei

$$H_n \Xi(\boldsymbol{R}_i) = E \Xi(\boldsymbol{R}_i) \tag{2–5}$$

where

$$H_n = \sum_{i} \frac{P_i}{2m_i} + U(\boldsymbol{R_i}) \tag{2–6}$$

This later equation does not contain any electronic degrees of freedom, because all electronic effects are incorporated into $U(\boldsymbol{R}_i)$ which is the interatomic potential. For molecular dynamics, Schrödinger's equation is replaced with Newton's equation of motion.

2.2 Empirical Interatomic Potentials

The interatomic potential $U(\boldsymbol{R}_i)$ derived from the Born-Oppenheimer approximation is derived from a quantum-mechanical perspective. The computational cost of *ab initio* such as density-functional theory (DFT) can provide accurate structural energies and forces, but their computational cost limits approaches to compute $U(\boldsymbol{R}_i)$ makes the scientific inquiry of systems requiring longer simulation times or larger number of atoms to captures relevant feature sizes unreasonable.

An empirical interatomic potential $V(\boldsymbol{R}_i; \boldsymbol{\theta})$ is an analytical function parameterized by $\boldsymbol{\theta} = (\theta_1, ..., \theta_n)$ which is meant to approximate $U(\boldsymbol{R}_i)$. The total energy of a potential of N atoms with an interaction described by the empirical potential, V, can be expanded in a many body expansion.

$$V(\boldsymbol{r}_1, ..., \boldsymbol{r}_N) = \sum_{i} V_1(\boldsymbol{r}_i) + \sum_{i}\sum_{i<j} V_2(\boldsymbol{r}_i, \boldsymbol{r}_j) + \sum_{i}\sum_{i<j}\sum_{j<k} V_3(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{r}_k) + ... \tag{2–7}$$

The first term V_1 is the one body term, due to an external field or boundary conditions, which is typically ignored in classical potentials. The second term V_2 is the pair potential, the interaction of the term is dependent upon the distance between $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$. The three-body term potential V_3 arises when the interaction interaction of a pair of atoms is modified by the presence of a third. Based upon this expansion, we can classify certain potentials into two classes: pair potentials when only V_2 is present and many-body potentials when V_3 and higher order terms are included.

2.2.1 Fitting Database

A fitting database is a collection of structure property functions q_i with an associated structures S_j. The notation of q comes from verification, validation, and uncertainty quantification literature where the term quantity of interest (QOI)

Lattice constant, bulk modulus, vacancy formation energy, or anything that can be defined from energy structures. In the fitting database, the structure proerty functions evaluated using an empirical potentials and compared to target reference values, with values either determined from experimental values or a a high-fidelity structure such as DFT.

The collection of structure property relationships, is denoted $\boldsymbol{q} = (q_1, q_2, ...q_N)$ for N structure property relationships. Usually accuracy and transferribility are tested against an external database.

2.2.2 Prediction Error function

In order to assess the prediction errors of the structure property functions, we denote the $\hat{\boldsymbol{q}}(\boldsymbol{\theta}) = (\hat{q}_1(\boldsymbol{\theta}), \hat{q}_2(\boldsymbol{\theta}), ..., \hat{q}_N(\boldsymbol{\theta}))$ as the predicted material properties

The difference between the prediction values and target values of the QOIs produces a vector of error functions, $\boldsymbol{\epsilon}(\boldsymbol{\theta}) = (\hat{q}_1(\boldsymbol{\theta}) - q_1, \hat{q}_2(\boldsymbol{\theta}) - q_2, ..., \hat{q}_N(\boldsymbol{\theta}) - q_N)$,

2.2.3 Cost Function

$$C(\boldsymbol{\theta}) = \sum w_i(\hat{q}_i(\boldsymbol{\theta}) - q_i)^2 \tag{2–8}$$

2.3 Notation

2.3.1 Simulation Cell

A simulation cell is defined by the lattice basis and the atomic basis. The lattice vectors which describes the periodic boundary conditions three lattice vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$Euclidean space which forms the basis for the crystallographic system when periodic boundary conditions are applied. The translational properties of a crystal allows the simulation of an infinite bulk material from a fixed volume. In traditional crystallography, the boundaries of the unit cell were defined as a, b, c corresponding to the length of each lattice vector and the angles α, β, γ. In computatonal materials, a more convenient representation

2.3.2

Let V be an empirical potential parameterized by P number of parameters $\boldsymbol{\theta} = [\theta_1, \theta_2, ...\theta_P]$. DEFINITION OF CONFIGURATION SPACE

The incorporation of first-principles data in the fitting database significantly improves the reliability of semi-empirical potentials by sampling a larger area of configuration space[21-28]

Ercolessi F, Adams JB. Europhys Lett 1994;26:583. Mishin Y, Farkas D, Mehl MJ, Papaconstantopoulos DA. Phys Rev B 1999;59:3393 Baskes MI, Asta M, Srinivasan SG. Philos Mag A 2001;81:991 Mishin Y, Mehl MJ, Papaconstantopoulos DA, Voter AF, Kress JD. Phys Rev B 2001;63:224106 Mishin Y, Mehl MJ, Papaconstantopoulos DA. Phys Rev B 2002;65:224114 Li Y, Siegel DJ, Adams JB, Liu XY. Phys Rev B 2003;67:125101 Zope RR, Mishin Y. Phys Rev B 2003;68:024102 Mishin Y. Acta Mater 2004;52:1451

CHAPTER 3
A PARETO APPROACH TO PARAMETER OPTIMIZATION

Many decision and plannning problems involve multiple conflicting criteria which must be considered simultaneously. In the field of optimization, problems which have multiple criteria are deferred to as multiple critieria decision making problems (MCDM) and the algorithms used to solve them as multiple-objective optimization (MOO).

Here the set of feasible solutons is not known in advance, but is restricted by constraint functions. We concentrate on nonlinear multiobjective optimization and ignore approaches designed for multiobjective linear programming.

Additionally, the approach described within this chapter is described briefly and is followed on by more detailed discussions and application in following chapters and appendices.

3.1 Multiobjective optimization

The general multi-objection optimization problem is posed as follows:

$$\begin{aligned} \underset{\boldsymbol{x}}{\text{minimize}} \quad & \boldsymbol{F}(\boldsymbol{x}) = [F_1(\boldsymbol{x}), F_2(\boldsymbol{x}), ..., F_k(\boldsymbol{x})]^T \\ \text{subject to} \quad & g_j(\boldsymbol{x}) \leq 0, j = 1, 2, ..., m \\ & h_l(\boldsymbol{x}) = 0, l =, 1, 2, ..., e \\ & \boldsymbol{x} \in \boldsymbol{X} \end{aligned} \tag{3–1}$$

where k is the number of objective functions, m is the number of inequality constraints, and e is the number of equality constraints. The vector $\boldsymbol{x} \in \boldsymbol{X} \subseteq \mathbb{R}^n$ is a vector design variables x_i, and X is feasible design space. $\boldsymbol{F}(\boldsymbol{x}) \in \mathbb{R}^k$ are called objectives, cost functions, or criteria. The feasible critereon space Z is defined as $\{\boldsymbol{F}(\boldsymbol{x}) | \boldsymbol{x} \in \boldsymbol{X}\}$ The emphasis of the development of this methdology will be on the mathematical aspects of the subject and it's applications to the development of classical empirical potentials. The intent is to provide tools for a decision maker, rather than to convince which particular optimization to use.

Secondly, another purpose of the development of this methdology is the development of parameterizations which can be expressed as an ensemble of potentials described as a probability distribution function which can be used in UQ propogation.

3.2 Pareto Front

In multiobjective optimization problems, it is characteristic that no unique solution exists, but a set of mathematically equally good solutions can be identified. These solutions are known as nondominated, efficient, noninferior or Pareto optimal solutions. In MCDM literature, these terms are synomous.

In MCDM literature, the idea of solving a multiobjective optimization problem is understood as helping a human decision maker (DM) in understanding the multiple objectives simultaneously and finding a Pareto optimal solution. Thus, the solution process requires some interaction with the DM in the form of specifying preference information and the final solution is determined by these preferences.

In potential development, the preferences of potential developer likewise influences are particular parameterization, which has results in the development of empirical potentials as somewhat of a black art. In the end, empirical potentials are simplified models which predict structure property relationships.

In classical potential optimization, the identification of an optimal parameterization is determined by the minimization of a cost function which couples multiple objective functions, usually a weighted sum of squares, and different weights are used in an interactive fashion until an acceptable parameterization is determined.

3.3 Surveys of Methods

Chankong and Haimes 1983 Hwang and Masud 1979 Marler and Arora 2004 Miettinen 1999 Sawaragi et al 1985 Steuer 1987 Vincke 1992

We start our review of methods using Hwang and Masud 1979 and Miettinen 199, to classify the different classes of approaches by methological approach rather than technical techniques.

3.3.1 no preference methods

The task is to find some neutral compromise solution without any additional information. This means instead of asking the DM for preference information, some assumption are made about what a reasonable compromise could be like.

3.3.2 *a priori* methods

In *a priori*, the DM first articulates preference information and the solution tries to find a Pareto optimal solution satisfying them as well as possible.

3.3.3 *a posteriori* methods

A representation of a set of Pareto optimal solution is first generated and then the DM is supposed to select the most preferred one among them. This approach gives the DM an overview of different solutions available but if there are more than two objectives in the problem, it may be difficult for the DM to analyze the large amount of information.

3.3.4 Interactive methods

After each iteration, some information is provided to the DM in order to specify preference information. What is noteworthy is that the DM can specify and adjust one's preferences between each iteration and at the same time learn about interdepencies between each iteration and at the same time learn about interdependencies in the problem as well as one's own preferences.

3.4 Solution Methods

MOO solution methods fall under the category of scalarization or non-scalarization methods. Scalarization is the primary method for MOO problems [Miettinen 1999]. Scalarization converts the MOO problem into a paramterized single-objective problem which can be solved using using well-established single-objective optimization methods.

3.4.1 Scalarization Methods

3.4.1.1 Weighting Method

Gass and Saaty 1955 Zadeh 1963

For a interatomic potential being fit with respect to k quantities of interest,

$$\begin{aligned} \underset{\boldsymbol{\theta}}{\text{minimize}} \quad & \sum_{i=1}^{k} w_i \varepsilon_i^2(\boldsymbol{\theta}) \\ \text{subject to} \quad & \boldsymbol{\theta} \in \boldsymbol{\Theta} \end{aligned} \tag{3–2}$$

where $w_i \geq 0$ for $i = 1, ..., k$ Weakly Pareto optimal.

In the development of interatomic potentials, the DM is asked to specify weights in which case the method is used as an *a priori* method.

Algorithms for multiobjective optimization should produce Pareto optimal solutions, and that any Pareto optimal solution can be found. Censor1977 discusses the conditions which the whole Pareto set can be generated by the weighting metho when positive weights are presented. In this respect, the weighting method has a serious shortcoming. Any Pareto optimal solution can be found by altering weights only if the problem is convex. Some Pareto optimal solutions of nonconvex problems cannot be found regardless of how the weights are selected.

The problems of the weighting schemes have ben explored by the classical potential development community. The method may jump from one vertex to anohter vertex leaving intermediate solutions undetected with relatively small changes in the weighting schemes.

Scaling of the objective functions.

The weighting method can be used as an *a posteriori* method where different weight can be used to generate different Pareto optimal solutions, and then the DM selects the most satisfactory solution. Systemic methods of perturbing the weights to obatain different Pareto optimal solutions are suggested (Chankong and Haimes 1983), but Das and Dennis 1997 illustrates that an evenly distributed set of weights does not necessarily produce an evenly distributed representation of the Pareto optimal set, even when the problem is convex.

When the weighting scheme is used as an *a priori* method, the DM is expected to represent his/her preferences in the form of weights. Roy and Mousseau (1996) suggests that the role of weights in expressing preferences maybe mis leading. Although the relative importance of weights show the relative importance of the objective functions it is not clear what underlies this notion. The relative importance of objective functions is usually understood globally, for the entire decision problem, while many practical applications show that the importannce typically varies for different objective function values, that is, the concept is only meaningful locally. (Podinovsky 1994).

Weights that produce a certain Pareto optimal solution are not necessarily unique, and different weights may produce similar solutions. On the other hand, a small change in weights may cause big differences in the objective function. It is not easy for the potential developer to control the solution process because weights behave in an indirect way. The solution process then becomes an interactive one where the DM trues to guess such weights that would produce a satisfactory solution, and this is not desirable because the DM cannot be properly suppported which leads to frustation complications in potential development. Instead, in such cases it is advisable to use real interactive methods where the DM can better control the solution process with more intuitive preference information.

The weighting method is also difficult https://books.google.com/books?id=NHZqCQAAQBAJpg=P
$4v = onepageqf = false$

3.5 Optimization Methods

$$\begin{aligned} \underset{\boldsymbol{x}}{\text{minimize}} \quad & f(x) \\ \text{subject to} \quad & g_i(x) \leq 0 \quad h_j(x) = 0 \quad x \in X \end{aligned} \tag{3–3}$$

here x is the optimization variable, f is the objective function, g_i are inequality constraints, and h_j are equality constraint functions.

3.5.1 Convex Optimization

Numerical algorithms make heavy use of scalarization results, and most papers in the field of MOO and economics deal with non-linear programming problems, corresponding duality theorems, and the repeated application of the simplex method.

However, within the literature of potential development approaches focus upon local minimization techniques and global optimization techniques.

objective function is concave. constraint set is convex. KKT requirements for uniqueness.

3.5.2

3.6 Visualization

This problem is dealt with in discussions about visualization and and analysis of the large amounts of data generated from a posteriori approaches to solving these problems. Edgeworth 1881 Koopmans 1951 Kuhn Tucker 1951 Pareto 1896, 1906

3.7 Treatment

Our treatment of the mapping of the empirical potential is treated as a bijective mapping into two measure spaces.

Let us define parameter space with the probability measure space $(\Theta, \mathcal{F}(\Theta), \mathbb{P})$.

Then we define the error space of the structure property relationships with the probability measure space $(\mathcal{E}, \mathcal{F}(\mathcal{E})), \mathbb{Q})$.

CHAPTER 4
RESULTS

4.1 Fusce Eget Tempus Lectus,

Algorithm 4.1. *Euclid's algorithm*

```
procedure Euclid(a, b)                        ▷ The g.c.d. of a and b
    r ← a mod b
    while r ≠ 0 do                            ▷ We have the answer if r is 0
        a ← b
        b ← r
        r ← a mod b
    end while
    return b                                  ▷ The gcd is b
end procedure
```

Proposition 4.1. *The Upsilon Function*

(1) If $\beta > 0$ and $\alpha \neq 0$, then for all $n \geq -1$,

$$I_n(c;\alpha;\beta;\delta) = -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^{n-i}Hh_i(\beta c-\delta)$$

$$+(\frac{\beta}{\alpha})^{n+1}\frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(-\beta c+\delta+\frac{\alpha}{\beta})$$

(2) If $\beta < 0$ and $\alpha < 0$, then for all $x \geq -1$

$$I_n(c;\alpha;\beta;\delta) = -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^{n-i}Hh_i(\beta c-\delta)$$

$$-(\frac{\beta}{\alpha})^{n+1}\frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(\beta c-\delta-\frac{\alpha}{\beta})$$

Proof. Case 1.

$\beta > 0$ and $\alpha \neq 0$. Since, for any constant α and $n \geq 0$, $e^{\alpha x}Hh_n(\beta x-\delta) \to 0$ as $x \to \infty$ thanks to (B4), integration by parts leads to

$$I_n = -\frac{1}{\alpha}Hh(\beta c-\delta)e^{\alpha c} + \frac{\beta}{\alpha}\int_c^{\infty} e^{\alpha x}Hh_{n-1}(\beta c-\delta)dx$$

In other words, we have a recursion, for $n \geq 0$, $I_n = -(e^{\alpha c}\alpha)Hh_n(\beta c - \delta) + (\frac{\beta}{\alpha})I_{n-1}$ with

$$I_{-1} = \sqrt{2\pi}\int_c \infty e^{\alpha x}\varphi(-\beta x + \delta)dx$$

$$= \frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(-\beta c + \delta + \frac{\alpha}{\beta})$$

Solving it yields, for $n \geq -1$,

$$I_n = -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^i Hh_{n-i}(\beta c + \delta) + (\frac{\beta}{\alpha})^{n+1}I_{-1}$$

$$= -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^{n-i}Hh_i(\beta c + \delta)$$

$$+(\frac{\beta}{\alpha})^{n+1}\frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(-\beta c + \delta + \frac{\alpha}{\beta})$$

where the sum over an empty set is defined to be zero. □

Proof. Case2. $\beta < 0$ and $\alpha < 0$. In this case, we must also have, for $n \geq 0$ and any constant $\alpha < 0, e^{\alpha x}Hh_n(\beta x - \delta) \to 0$ as

$x \to \infty$, thanks to (B5). Using integration by parts, we again have the same recursion, for $n \geq 0, I_n = -(e^{\alpha c}/\alpha)Hh_n(\beta c - \delta) + (\beta/\alpha)I_{n-1}$, but with a different initial condition

$$I_{-1} = \sqrt{2\pi}\int_c^{\infty} e^{\alpha x}\varphi(-\beta x + \delta)dx$$

$$= -\frac{\sqrt{2\pi}}{\beta}exp\{\frac{\alpha\delta}{\beta} + \frac{\alpha^2}{2\beta^2}\}\phi(\beta c - \delta - \frac{\alpha}{\beta})$$

Solving it yields (B8), for $n \geq -1$.

□

Finally, we sum the double exponential and the normal random variables

Proposition B.3.

Suppose $\{\xi_1, \xi_2, ...\}$ *is a sequence of i.i.d. exponential random variables with rate* $\eta > 0$*, and* Z *is a normal variable with distribution* $N(0, \sigma^2)$*. Then for every* $n \geq 1$*, we have: (1) The density functions are given by:*

$$f_{Z+\sum_{i=1}^n \xi_i}(t) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} Hh_{n-1}(-\frac{t}{\sigma} + \sigma\eta)$$

$$f_{Z-\sum_{i=1}^n \xi_i}(t) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} Hh_{n-1}(\frac{t}{\sigma} + \sigma\eta)$$

(2) The tail probabilities are given by

$$P(Z + \sum_{i=1}^n \xi_i \geq x) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} I_{n-1}(x; -\eta, -\frac{1}{\sigma}, -\sigma\eta)$$

$$P(Z - \sum_{i=1}^n \xi_i \geq x) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} I_{n-1}(x; \eta, \frac{1}{\sigma}, -\sigma\eta)$$

Proof. Case 1. The densities of $Z + \sum_{i=1}^n \xi_i$*, and* $Z - \sum_{i=1}^n \xi_i$*. We have*

$$f_{Z+\sum_{i=1}^n \xi_i}(t) = \int_{-\infty}^{\infty} f_{\sum_{i=1}^n \xi_i}(t-x) f_Z(x) dx$$

$$= e^{-t\eta}(\eta^n) \int_{-\infty} t \frac{e^{x\eta}(t-x)^{n-1}}{(n-1)!} \frac{1}{\sigma\sqrt{2\pi}} e^{-x^2/(2\sigma^2)} dx$$

$$= e^{-t\eta}(\eta^n) e^{(\sigma\eta)^2/(2)} \int_{-\infty} t \frac{(t-x)^{n-1}}{(n-1)!} \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\sigma^2\eta)^2/(2\sigma^2)} dx$$

Letting $y = (x - \sigma^2\eta)/\sigma$ *yields*

$$f_{Z+\sum_{i=1}^n \xi_i}(t) = e^{-t\eta}(\eta^n) e^{(\sigma\eta)^2/(2)} \sigma^{n-1}$$

$$\times \int_{-\infty}^{t/\sigma-\sigma\eta} \frac{(t/\sigma - y - \sigma\eta)^{n-1}}{(n-1)!} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} dy$$

$$= \frac{e^{(\sigma\eta)^2/2}}{\sqrt{2\pi}} (\sigma^{n-1}\eta^n) e^{-t\eta} Hh_{n-1}(-t/\sigma + \sigma\eta)$$

because $(1/(n-1)!) \int_{-\infty} a(a-y)^{n-1} e^{-y^2/2} dy = Hh_{n-1}(a)$. *The derivation of* $f_{Z+\sum_{i=1}^n \xi_i}(t)$ *is similar.*

Case 2. $P(Z + \sum_{i=1}^n \xi_i \geq x)$ *and* $P(Z - \sum_{i=1}^n \xi_i \geq x)$. *From (B9), it is clear that*

$$P(Z + \sum_{i=1}^n \xi_i \geq x) = \frac{(\sigma\eta)^n e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} \int_x^\infty e^{(-i\eta)} Hh_{n-1}(-\frac{t}{\sigma} + \sigma\eta) dt$$

$$= \frac{(\sigma\eta)^n e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} I_{n-1}(x; -\eta, -\frac{1}{\sigma}, -\sigma\eta) dt$$

by (B6). We can compute $P(Z - \sum_{i=1}^n \xi_i \geq x)$ *similarly.*

Theorem 4.1. *Theorem With* $\pi_n := P(N(t) = n) = e^{-\lambda T}(\lambda T)^n/n!$ *and* I_n *in Proposition* **??**. *, we have*

$$P(Z(T) \geq a) = \frac{e^{(\sigma\eta_1)^2 T/2}}{\sigma\sqrt{2\pi T}} \sum_{n=1}^\infty \pi_n \sum_{k=1}^n P_{n,k} (\sigma\sqrt{T}\eta_1)^k \times I_{k-1}(a - \mu T; -\eta_1, -\frac{1}{\sigma\sqrt{T}}, -\sigma\eta_1\sqrt{T})$$

$$+ \frac{e^{(\sigma\eta_2)^2 T/2}}{\sigma\sqrt{2\pi T}} \sum_{n=1}^\infty \pi_n \sum_{k=1}^n Q_{n,k} (\sigma\sqrt{T}\eta_2)^k$$

$$\times I_{k-1}(a - \mu T; \eta_2, \frac{1}{\sigma\sqrt{T}}, -\sigma\eta_2\sqrt{T})$$

$$+ \pi_0 \phi(-\frac{a - \mu T}{\sigma\sqrt{T}})$$

Proof by the decomposition (B2)

$$P(Z(T) \geq a) = \sum_{n=0}^{\infty} \pi_n P(\mu T + \sigma\sqrt{T} Z + \sum_{j=1}^{n} Y_j \geq a)$$

$$= \pi_0 P(\mu T + \sigma\sqrt{T} Z \geq a)$$

$$+ \sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} P_{n,k} P(\mu T + \sigma\sqrt{T} Z + \sum_{j=1}^{n} \xi_j^{+} \geq a)$$

$$+ \sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} Q_{n,k} P(\mu T + \sigma\sqrt{T} Z - \sum_{j=1}^{n} \xi_j^{-} \geq a)$$

The result now follows via (B11) and (B12) for $\eta_1 > 1$ *and* $\eta_2 > 0$.

CHAPTER 5
SUMMARY AND CONCLUSIONS

5.1 Non Porttitor Tellus

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APPENDIX A
THIS IS THE FIRST APPENDIX

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APPENDIX B
AN EXAMPLE OF A HALF TITLE PAGE

LaTeX 2_{ε}

Figure B-1. LaTeX2ϵ. logo

This is how a section should look if the first page is a landscape page. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut sit amet nulla. Integer mauris turpis, dapibus ac, auctor non, vehicula sit amet, magna. Suspendisse eu tellus. Etiam porta. Donec magna. Donec ut dui. In hac habitasse platea dictumst. Nullam suscipit, mi at adipiscing commodo, lorem erat scelerisque erat, non pulvinar leo mi eu metus. Phasellus id felis. Sed quam purus, molestie quis, ultrices nec, dictum at, magna. Proin viverra viverra ante.

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APPENDIX C
DERIVATION OF THE Υ FUNCTION

Proposition C.1. *The Upsilon Function*

(1) If $\beta > 0$ and $\alpha \neq 0$, then for all $n \geq -1$,

$$I_n(c;\alpha;\beta;\delta) = -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^{n-i}Hh_i(\beta c - \delta)$$

$$+(\frac{\beta}{\alpha})^{n+1}\frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(-\beta c + \delta + \frac{\alpha}{\beta})$$

(2) If $\beta < 0$ and $\alpha < 0$, then for all $x \geq -1$

$$I_n(c;\alpha;\beta;\delta) = -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^{n-i}Hh_i(\beta c - \delta)$$

$$-(\frac{\beta}{\alpha})^{n+1}\frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(\beta c - \delta - \frac{\alpha}{\beta})$$

Proof. Case 1.

$\beta > 0$ and $\alpha \neq 0$. Since, for any constant α and $n \geq 0$, $e^{\alpha x}Hh_n(\beta x - \delta) \to 0$ as $x \to \infty$ thanks to (B4), integration by parts leads to

$$I_n = -\frac{1}{\alpha}Hh(\beta c - \delta)e^{\alpha c} + \frac{\beta}{\alpha}\int_c^{\infty} e^{\alpha x}Hh_{n-1}(\beta c - \delta)dx$$

In other words, we have a recursion, for $n \geq 0$, $I_n = -(e^{\alpha c}\alpha)Hh_n(\beta c - \delta) + (\frac{\beta}{\alpha})I_{n-1}$ with

$$I_{-1} = \sqrt{2\pi}\int_c \infty e^{\alpha x}\varphi(-\beta x + \delta)dx$$

$$= \frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(-\beta c + \delta + \frac{\alpha}{\beta})$$

Solving it yields, for $n \geq -1$,

$$I_n = -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^i Hh_{n-i}(\beta c+\delta) + (\frac{\beta}{\alpha})^{n+1} I_{-1}$$

$$= -\frac{e^{\alpha c}}{\alpha}\sum_{i=0}^{n}(\frac{\beta}{\alpha})^{n-i} Hh_i(\beta c+\delta)$$

$$+(\frac{\beta}{\alpha})^{n+1}\frac{\sqrt{2\pi}}{\beta}e^{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}}\phi(-\beta c+\delta+\frac{\alpha}{\beta})$$

where the sum over an empty set is defined to be zero. □

Case2. $\beta < 0$ and $\alpha < 0$. In this case, we must also have, for $n \geq 0$ and any constant $\alpha < 0, e^{\alpha x} Hh_n(\beta x - \delta) \to 0$ as

$x \to \infty$, thanks to (B5). Using integration by parts, we again have the same recursion, for $n \geq 0, I_n = -(e^{\alpha c}/\alpha)Hh_n(\beta c - \delta) + (\beta/\alpha)I_{n-1}$, but with a different initial condition

$$I_{-1} = \sqrt{2\pi}\int_c^{\infty} e^{\alpha x}\varphi(-\beta x+\delta)dx$$

$$= -\frac{\sqrt{2\pi}}{\beta}exp\{\frac{\alpha\delta}{\beta}+\frac{\alpha^2}{2\beta^2}\}\phi(\beta c-\delta-\frac{\alpha}{\beta})$$

Solving it yields (B8), for $n \geq -1$.

Finally, we sum the double exponential and the normal random variables

Proposition B.3.

Suppose $\{\xi_1, \xi_2, ...\}$ is a sequence of i.i.d. exponential random variables with rate $\eta > 0$, and Z is a normal variable with distribution $N(0, \sigma^2)$. Then for every $n \geq 1$, we have: (1) The density functions are given by:

$$f_{Z+\sum_{i=1}^{n}\xi_i}(t) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}}e^{-t\eta}Hh_{n-1}(-\frac{t}{\sigma}+\sigma\eta)$$

$$f_{Z-\sum_{i=1}^{n}\xi_i}(t) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}}e^{-t\eta}Hh_{n-1}(\frac{t}{\sigma}+\sigma\eta)$$

(2) The tail probabilities are given by

$$P(Z+\sum_{i=1}^{n}\xi_i \geq x) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} I_{n-1}(x; -\eta, -\frac{1}{\sigma}, -\sigma\eta)$$

$$P(Z-\sum_{i=1}^{n}\xi_i \geq x) = (\sigma\eta)^n \frac{e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} e^{-t\eta} I_{n-1}(x; \eta, \frac{1}{\sigma}, -\sigma\eta)$$

Proof. Case 1. The densities of $Z+\sum_{i=1}^{n}\xi_i$, *and* $Z-\sum_{i=1}^{n}\xi_i$. *We have*

$$f_{Z+\sum_{i=1}^{n}\xi_i}(t) = \int_{-\infty}^{\infty} f_{\sum_{i=1}^{n}\xi_i}(t-x) f_Z(x) dx$$

$$= e^{-t\eta}(\eta^n) \int_{-\infty} t \frac{e^{x\eta}(t-x)^{n-1}}{(n-1)!} \frac{1}{\sigma\sqrt{2\pi}} e^{-x^2/(2\sigma^2)} dx$$

$$= e^{-t\eta}(\eta^n) e^{(\sigma\eta)^2/(2)} \int_{-\infty} t \frac{(t-x)^{n-1}}{(n-1)!} \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\sigma^2\eta)^2/(2\sigma^2)} dx$$

Letting $y = (x-\sigma^2\eta)/\sigma$ *yields*

$$f_{Z+\sum_{i=1}^{n}\xi_i}(t) = e^{-t\eta}(\eta^n) e^{(\sigma\eta)^2/(2)} \sigma^{n-1}$$

$$\times \int_{-\infty}^{t/\sigma-\sigma\eta} \frac{(t/\sigma-y-\sigma\eta)^{n-1}}{(n-1)!} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} dy$$

$$= \frac{e^{(\sigma\eta)^2/2}}{\sqrt{2\pi}} (\sigma^{n-1}\eta^n) e^{-t\eta} Hh_{n-1}(-t/\sigma+\sigma\eta)$$

because $(1/(n-1)!) \int_{-\infty} a(a-y)^{n-1} e^{-y^2/2} dy = Hh_{n-1}(a)$. *The derivation of* $f_{Z+\sum_{i=1}^{n}\xi_i}(t)$ *is similar.*

Case 2. $P(Z+\sum_{i=1}^{n}\xi_i \geq x)$ *and* $P(Z-\sum_{i=1}^{n}\xi_i \geq x)$. *From (B9), it is clear that*

$$P(Z+\sum_{i=1}^{n}\xi_i \geq x) = \frac{(\sigma\eta)^n e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} \int_x^{\infty} e^{(-i\eta)} Hh_{n-1}(-\frac{t}{\sigma}+\sigma\eta) dt$$

$$= \frac{(\sigma\eta)^n e^{(\sigma\eta)^2/2}}{\sigma\sqrt{2\pi}} I_{n-1}(x; -\eta, -\frac{1}{\sigma}, -\sigma\eta)dt$$

by (B6). We can compute $P(Z - \sum_{i=1}^n \xi_i \geq x)$ similarly.

Theorem C.1. *Theorem With $\pi_n := P(N(t) = n) = e^{-\lambda T}(\lambda T)^n/n!$ and I_n in Proposition* **??**. *, we have*

$$P(Z(T) \geq a) = \frac{e^{(\sigma\eta_1)^2 T/2}}{\sigma\sqrt{2\pi T}} \sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} P_{n,k}(\sigma\sqrt{T}\eta_1)^k \times I_{k-1}(a - \mu T; -\eta_1, -\frac{1}{\sigma\sqrt{T}}, -\sigma\eta_1\sqrt{T})$$

$$+\frac{e^{(\sigma\eta_2)^2 T/2}}{\sigma\sqrt{2\pi T}} \sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} Q_{n,k}(\sigma\sqrt{T}\eta_2)^k$$

$$\times I_{k-1}(a - \mu T; \eta_2, \frac{1}{\sigma\sqrt{T}}, -\sigma\eta_2\sqrt{T})$$

$$+\pi_0\phi(-\frac{a - \mu T}{\sigma\sqrt{T}})$$

Proof by the decomposition (B2)

$$P(Z(T) \geq a) = \sum_{n=0}^{\infty} \pi_n P(\mu T + \sigma\sqrt{T}Z + \sum_{j=1}^{n} Y_j \geq a)$$

$$= \pi_0 P(\mu T + \sigma\sqrt{T}Z \geq a)$$

$$+\sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} P_{n,k} P(\mu T + \sigma\sqrt{T}Z + \sum_{j=1}^{n} \xi_j^+ \geq a)$$

$$+\sum_{n=1}^{\infty} \pi_n \sum_{k=1}^{n} Q_{n,k} P(\mu T + \sigma\sqrt{T}Z - \sum_{j=1}^{n} \xi_j^- \geq a)$$

The result now follows via (B11) and (B12) for $\eta_1 > 1$ and $\eta_2 > 0$.

APPENDIX D
DERIVATION OF THE Υ FUNCTION

We first decompose the sum of the double exponential random variables.

The memoryless property of exponential random variables yields $(\xi^+ - \xi^- | \xi^+ > \xi^-) =^d \xi^+$ and $(\xi^+ - \xi^- | \xi^+ < \xi^-) =^d -\xi^-$, thus leading to the conclusion that

$$\xi^+ - \xi^- = \left\{ \begin{array}{rl} \xi^+ & \text{with probability } \eta_2/(\eta_1+\eta_2) \\ -\xi^- & \text{with probability } \eta_1/(\eta_1+\eta_2) \end{array} \right\}.$$

because the probabilities of the events $\xi^+ > \xi^-$ and $\xi^+ < \xi^-$ are $\eta_2/(\eta_1+\eta_2)$ and $\eta_1/(\eta_1+\eta_2)$, respectively. The following proposition extends (B.1.)

Proposition B.1. For every $n \geq 1$, we have the following decomposition

$$\sum_{i=1}^{n} Y_i =^d \left\{ \begin{array}{rl} \sum_{i=1}^{k} \xi_i^+ & \text{with probability } P_{n,k}, k = 1, 2, ..., n \\ -\sum_{i=1}^{k} \xi_i^- & \text{with probability } Q_{n,k}, k = 1, 2, ..., n \end{array} \right\}.$$

where $P_{n,k}$ and $Q_{n,k}$ are given by

$$P_{n,k} = \sum_{i=k}^{n-1} \binom{n-k-1}{i-k} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{i-k} (\frac{\eta_2}{\eta_1+\eta_2})^{n-i} p^i q^{n-i}$$

$$1 \leq k \leq n-1$$

$$Q_{n,k} = \sum_{i=k}^{n-1} \binom{n-k-1}{i-k} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{n-i} (\frac{\eta_2}{\eta_1+\eta_2})^{i-k} p^{n-i} q^i$$

$$1 \leq k \leq n-1, P_{n,n} = p^n, Q_{n,n} = q^n$$

and $\binom{0}{0}$ is defined to be one. Hence ξ_i^+ and ξ_i^- are i.i.d. exponential random variables with rates η_1 and η_2, respectively.

As a key step in deriving closed-form solutions for call and put options, this proposition indicates that the sum of the i.i.d. double exponential random variable can be written, in distribution, as a randomly mixed gamma random variable. To prove Proposition B.1, the following lemma is needed.

Lemma B.1.

$$\sum_{i=1}^{n} \xi_i^+ - \sum_{i=1}^{n} \xi_i^-$$

$$=^d \left\{ \begin{array}{ll} \sum_{i=1}^{k} \xi_i & \text{with probability } \binom{n-k+m-1}{m-1}(\frac{\eta_1}{\eta_1+\eta_2})^{n-k}(\frac{\eta_2}{\eta_1+\eta_2})^{m}, k = 1, ..., n \\ -\sum_{i=1}^{l} \xi_i & \text{with probability } \binom{n-l+m-1}{n-1}(\frac{\eta_1}{\eta_1+\eta_2})^{n}(\frac{\eta_2}{\eta_1+\eta_2})^{m-l}, l = 1, ..., m \end{array} \right\}.$$

We prove it by introducing the random variables $A(n,m) = \sum_{i=1}^{n} \xi_i - sum_{j=1}^{m} \tilde{\xi}_j$ Then

$$A(n,m) =^d \left\{ \begin{array}{ll} A(n-1,m-1) + \xi^+ & \text{with probability } \eta_2/(\eta_1+\eta_2) \\ A(n-1,m-1) - \xi^- & \text{with probability } \eta_1/(\eta_1+\eta_2) \end{array} \right\}.$$

$$=^d \left\{ \begin{array}{ll} A(n,m-1) & \text{with probability } \eta_2/(\eta_1+\eta_2) \\ A(n-1,m) & \text{with probability } \eta_1/(\eta_1+\eta_2) \end{array} \right\}.$$

via B.1.. Now suppose horizontal axis that are representing the number of $\{\zeta_i^+\}$ and vertical axis representing the number of $\{\zeta_i^-\}$. Suppose we have a random walk on the integer lattice points. Starting from any point $(n,m), n, m \geq 1$, the random walk goes either one step to the left with probability $\eta_1/(\eta_1+\eta_2)$ or one step down with probability $\eta_2/(\eta_1+\eta_2)$, and the random walks stops once it reaches the horizontal or vertical axis. For any path from (n,m) to (k,0) , $1 \geq k \geq n$, it must reach (k,1) first before it makes a final move to (k,0). Furthermore, all the paths going from (n,m) to (k,1) must have exactly n-k lefts and m-1 downs, whence the total number of such paths is $\binom{n-k+m-1}{m-1}$. Similarly the total number of paths from (n,m) to (0,l) , $1 \geq l \geq m$, is $\binom{n-l+m-1}{n-1}$. Thus

$$A(n,m) =^d \left\{ \begin{array}{ll} \sum_{i=1}^{k} \xi_i & \text{with probability } \binom{n-k+m-1}{m-1}(\frac{\eta_1}{\eta_1+\eta_2})^{n-k}(\frac{\eta_2}{\eta_1+\eta_2})^m, k = 1, ..., n \\ -\sum_{i=1}^{l} \xi_i & \text{with probability } \binom{n-l+m-1}{n-1}(\frac{\eta_1}{\eta_1+\eta_2})^{n}(\frac{\eta_2}{\eta_1+\eta_2})^{m-l}, l = 1, ..., m \end{array} \right\}.$$

and the lemma is proven.

Now, let's prove the proposition B.1. By the same analogy used in Lemma B.1 to compute probability $P_{n,m}, 1 \geq k \geq n$, the probability weight assigned to $\sum_{i=1}^{k} \xi_i^+$ when we decompose $\sum_{i=1}^{k} Y_i$, it is equivalent to consider the probability of the random walk ever reach (k,0) starting from the point (i,n-i) being $\binom{n}{i} p^i q^{n-i}$. Note that the point (k,0) can only be reached from point (i,n-i) such that $k \geq i \geq n-1$, because the random walk can only go left or down, and stops once it reaches the horizontal axis. Therefore, for $1 \geq k \geq n-1$, (B3) leads to

$$P_{n,k} = \sum_{i=k} n - 1P(goingfrom(i,n-i)to(k,0)).P(startingfrom(i,n-i))$$

$$= \sum_{i=k}^{n-1} \binom{i+(n-i)-k-1}{(n-i)-1} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{i-k} (\frac{\eta_2}{\eta_1+\eta_2})^{n-i} p^i q^{n-i}$$

$$= \sum_{i=k}^{n-1} \binom{n-k-1}{n-i-1} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{i-k} (\frac{\eta_2}{\eta_1+\eta_2})^{n-i} p^i q^{n-i}$$

$$= \sum_{i=k}^{n-1} \binom{n-k-1}{i-k} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{i-k} (\frac{\eta_2}{\eta_1+\eta_2})^{n-i} p^i q^{n-i}$$

Of course $P_{n,n} = p^n$. Similarly, we can compute $Q_{n,k}$:

$$Q_{n,k} = \sum_{i=k} n - 1P(goingfrom(n-i,i)to(0,k)).P(startingfrom(n-i,i))$$

$$= \sum_{i=k}^{n-1} \binom{i+(n-i)-k-1}{(n-i)-1} \binom{n}{n-i} (\frac{\eta_1}{\eta_1+\eta_2})^{n-i} (\frac{\eta_2}{\eta_1+\eta_2})^{i-k} p^{n-i} q^i$$

$$= \sum_{i=k}^{n-1} \binom{n-k-1}{i-k} \binom{n}{i} (\frac{\eta_1}{\eta_1+\eta_2})^{n-i} (\frac{\eta_2}{\eta_1+\eta_2})^{i-k} p^{n-i} q^i$$

with $Q_{n,n} = q^n$. Incidentally, we have also got $\sum k = 1n(P_{n,k} + Q_{n,k}) = 1$

B.2. Let's develop now the results on Hh functions. First of all, note that $Hh_n(x) \to 0$, as $x \to \infty$, for $n \geq -1$; and $Hh_n(x) \to \infty$, as $x \to -\infty$, for $n \geq -1$; and $Hh_0(x) = \sqrt{2\pi}\phi(-x) \to \sqrt{2\pi}$, as $x \to -\infty$. Also, for every $n \geq -1$, as $x \to \infty$,

$$lim Hh_n(x) / \{\frac{1}{x^{n+1}} e^{-\frac{x^2}{2}}\} = 1$$

and as $x \to \infty$

$$Hh_n(x) = O(|x|^n)$$

Here (B4) is clearly true for $n = -1$, while for $n \geq 0$ note that as $x \to_\infty$,

$$Hh_n(x) = \frac{1}{n!} \int_x \infty (t-x)^n e^{-\frac{t^2}{2}} dt$$

$$\leq \frac{2^n}{n!} \int_{-\infty}^{\infty} |t|^n e^{-t^2} 2dt + \frac{2^n}{n!} \int -\infty\infty |x|^n e^{-t^2} 2dt = O(|x|^n)$$

For option pricing it is important to evaluate the integral $I_n(c; \alpha; \beta; \delta)$,

$$I_n(c; \alpha; \beta; \delta) = \int_c \infty e^{\alpha x} Hh_n(\beta x - \delta) dx, n \geq 0$$

for arbitrary constants α, c and β.

REFERENCES

[1] K. L. Green, “A wrinkle in time,” *comiXology*, 2008.

[2] H. D. Strickler, P. S. Rosenberg, S. S. Devesa, J. Hertel, J. F. Fraumeni Jr, and J. J. Goedert, “Contamination of poliovirus vaccines with simian virus 40 (1955-1963) and subsequent cancer rates,” *Jama*, vol. 279, no. 4, pp. 292–295, 1998.

[3] M. L’engle, *A Wrinkle in Time: 50th Anniversary Commemorative Edition.* Macmillan, 2012, vol. 1.

[4] D. Garfinkle, G. T. Horowitz, and A. Strominger, “Charged black holes in string theory,” *Physical Review D*, vol. 43, no. 10, p. 3140, 1991.

BIOGRAPHICAL SKETCH

This section is where your biographical sketch is typed in the bio.tex file. It should be in third person, past tense. Do not put personal details such as your birthday in the file. Again, to make a full paragraph you must write at least three sentences.