CRANFIELD UNIVERSITY

Mateusz Golab

Forward integration of simultaneous ordinary differential equations with graphical output

School of Engineering

Software Engineering for Technical Computing

MSc THESIS

Academic Year: 2011 - 2012

Supervisor: Dr Peter Sherar, Prof Joanna Polanska

August 2012

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Supervisor: Dr Peter Sherar, Prof Joanna Polanska

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This thesis is submitted in partial fulfilment of the requirements for the degree of Master of Science

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ABSTRACT

Ordinary differential equations are used to model physical and mathematical systems that evolve over time. ODEs are present in many branches of science especially in pure and applied mathematics. Many models base on these equations, so efficient solving methods are essential.

The investigation of numerical routines for solving ODE’s is presented in this report. It comprises of explanation and comparison of most efficient practical numerical methods available.

This thesis report contains also description of design, testing and implementation of web application based on AJAX technologies, solving systems of ordinary differential equations. Moreover application devises 2D graphical representation of a solution and enables user to store and load systems of ODE’s. Part of this report is dedicated to technologies used to develop the application, with emphasis on Google Web Toolkit and Google AppEngine . Moreover, details of software lifecycle model and agile approaches used are pointed as well.

Finally, numerical methods and technologies choices are discussed . Additional analysis is provided for application’s results along with problems faced during development process. The final conclusion is followed by ideas of future improvements.

Keywords:

ODE, Runge-Kutta, Modified Midpoint, Adams-Bashforth-Moulton, Web development, GWT, AppEngine, Datastore, Unit testing, Test Driven Development, Prototyping

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TABLE OF CONTENTS

[ABSTRACT i](#_Toc333002832)

[ACKNOWLEDGEMENTS iii](#_Toc333002833)

[LIST OF FIGURES vii](#_Toc333002834)

[LIST OF TABLES viii](#_Toc333002835)

[LIST OF EQUATIONS ix](#_Toc333002836)

[LIST OF ABBREVIATIONS xi](#_Toc333002837)

[1. Introduction 1](#_Toc333002838)

[1.1 Overview 1](#_Toc333002839)

[1.2 Aims and objectives 1](#_Toc333002840)

[1.3 Motivation 2](#_Toc333002841)

[1.4 Literature review 2](#_Toc333002842)

[1.5 Thesis structure 3](#_Toc333002843)

[2 Mathematical background 5](#_Toc333002844)

[2.1 Ordinary differential equations 5](#_Toc333002845)

[2.2 Euler’s method 6](#_Toc333002846)

[2.3 ODE numerical routines 6](#_Toc333002847)

[2.3.1 Runge-Kutta methods 6](#_Toc333002848)

[2.3.2 The modified midpoint 10](#_Toc333002849)

[2.3.3 Richardson extrapolation 11](#_Toc333002850)

[2.3.4 Rosenbrock 13](#_Toc333002851)

[2.3.5 Predictor- Corrector 14](#_Toc333002852)

[3 Technologies, Methodologies and Application Design 17](#_Toc333002853)

[3.1 AJAX approach 17](#_Toc333002854)

[3.2 Technologies used 18](#_Toc333002855)

[3.2.1 Google Web Toolkit 19](#_Toc333002856)

[3.2.2 Google AppEngine 20](#_Toc333002857)

[3.2.3 Datastore 21](#_Toc333002858)

[3.2.4 App Engine Administration console 23](#_Toc333002859)

[3.3 Architecture 23](#_Toc333002860)

[3.4 Design patterns 24](#_Toc333002861)

[3.5 The Prototyping Model 26](#_Toc333002862)

[3.6 Agile approach 27](#_Toc333002863)

[3.6.1 Feature Driven Development 27](#_Toc333002864)

[3.6.2 Test Driven Development 27](#_Toc333002865)

[3.7 Software versioning 28](#_Toc333002866)

[4 Testing 29](#_Toc333002867)

[4.1 Unit testing 29](#_Toc333002868)

[4.1.1 GWT Unit Testing infrastructure 29](#_Toc333002869)

[4.1.2 TDD approach 29](#_Toc333002870)

[4.1.3 Test Cases 30](#_Toc333002871)

[4.2 Black-Box testing 34](#_Toc333002872)

[4.2.1 Persistence tests 35](#_Toc333002873)

[5 Implementation 37](#_Toc333002874)

[5.1 The anatomy of the project 37](#_Toc333002875)

[5.2 Model 38](#_Toc333002876)

[5.2.1 Equation 38](#_Toc333002877)

[5.2.2 System 38](#_Toc333002878)

[5.2.3 SystemEntity 39](#_Toc333002879)

[5.2.4 Solution 39](#_Toc333002880)

[5.3 Equation Parser 40](#_Toc333002881)

[5.3.1 ParserServiceImpl 40](#_Toc333002882)

[5.4 ODE Solvers 41](#_Toc333002883)

[5.4.1 Solver base class 41](#_Toc333002884)

[5.4.2 ODE Solver services 41](#_Toc333002885)

[5.5 Graph Viewer 42](#_Toc333002886)

[5.6 Equation Store 42](#_Toc333002887)

[5.7 User interface 43](#_Toc333002888)

[5.7.1 Input Panel 43](#_Toc333002889)

[5.7.2 Equation Panel 44](#_Toc333002890)

[5.7.3 Graph Panel 45](#_Toc333002891)

[5.7.4 Equation Store GUI components 46](#_Toc333002892)

[5.7.5 Errors handling 46](#_Toc333002893)

[6 Results 47](#_Toc333002894)

[6.1 Parser Test Case results 47](#_Toc333002895)

[6.2 Solver Test Cases 47](#_Toc333002896)

[6.2.1 RungeKuttaSolverTestCase results 48](#_Toc333002897)

[6.2.2 ModifiedMidpointSolverTestCase results 49](#_Toc333002898)

[6.2.3 AdamsBashforthMoultonTestCase results 50](#_Toc333002899)

[7 Discussion and conclusion 51](#_Toc333002900)

[7.1 Analysis of numerical methods 51](#_Toc333002901)

[7.2 Analysis of application’s architecture 52](#_Toc333002902)

[7.3 Results analysis 53](#_Toc333002903)

[7.4 Problems faced 53](#_Toc333002904)

[7.5 Conclusion 54](#_Toc333002905)

[7.6 Future work 54](#_Toc333002906)

[REFERENCES 56](#_Toc333002907)

[APPENDICES 59](#_Toc333002908)

# LIST OF FIGURES

[Figure 2‑1 4th Order Runge-Kutta method 8](#_Toc333002909)

[Figure 2‑2 Richardson extrapolation used in the Burlisch-Stoer method with substep n = 2,4,6 [19] 12](#_Toc333002910)

[Figure 2‑3 Aitkens-Neville polynomial extrapolation tableau [19] 13](#_Toc333002911)

[Figure 3‑1 Comparison of AJAX light traffic needs versus legacy HTML applications [15] 18](#_Toc333002912)

[Figure 3‑2 An overview of GWT approach 19](#_Toc333002913)

[Figure 3‑3 Application architecture overview 24](#_Toc333002914)

[Figure 3‑4 Example of Command Pattern structure [21] 25](#_Toc333002915)

[Figure 3‑5 Example of Composite Pattern structure [22] 25](#_Toc333002916)

[Figure 3‑6 The prototyping lifecycle 26](#_Toc333002917)

[Figure 3‑7 Test Driven Development cycle 28](#_Toc333002918)

[Figure 5‑1 Input Panel 44](#_Toc333002919)

[Figure 5‑2 Equation Panel with example of ODE's system 45](#_Toc333002920)

[Figure 5‑3 2D graph presenting solution of sample system of ODE's 45](#_Toc333002921)

[Figure 5‑4 Developed dialog for loading systems of equations 46](#_Toc333002922)

[Figure 5‑5 Developed dialog for saving systems of equations 46](#_Toc333002923)

[Figure 5‑6 Example error dialog 46](#_Toc333002924)

[Figure 6‑1 ParserTestCase results 47](#_Toc333002925)

[Figure 6‑2 Runge Kutta TestCase results 48](#_Toc333002926)

[Figure 6‑3 Modified Midpoint TestCase results 49](#_Toc333002927)

[Figure 6‑4 Adams Bashforth Moulton TestCase results 50](#_Toc333002928)

LIST OF TABLES

[Table 3‑1 Datastore limitations 22](#_Toc333002929)

[Table 4‑1 Parser Test Case : correct ODE’s 30](#_Toc333002930)

[Table 4‑2 Parser Test Case : incorrect ODE’s 30](#_Toc333002931)

[Table 4‑3 Parser Test Case : equation’s incorrect variables 31](#_Toc333002932)

[Table 4‑4 Parser Test Case : case sensitivity 31](#_Toc333002933)

[Table 4‑5 Parser Test Case part 7 31](#_Toc333002934)

[Table 4‑6 Parser Test Case : initial values 32](#_Toc333002935)

[Table 4‑7 Parser Test Case : system of ODE's 32](#_Toc333002936)

[Table 4‑8 Solver Test Case : 1st order linear ODE 33](#_Toc333002937)

[Table 4‑9 Solver Test Case : 1st order non-linear ODE 33](#_Toc333002938)

[Table 4‑10 Solver Test Case : 1st order system of ODE's 34](#_Toc333002939)

LIST OF EQUATIONS

[(2‑1) 5](#_Toc333002940)

[(2‑2) 5](#_Toc333002941)

[(2‑3) 6](#_Toc333002942)

[(2‑4) 6](#_Toc333002943)

[(2‑5) 6](#_Toc333002944)

[(2‑6) 6](#_Toc333002945)

[(2‑7) 7](#_Toc333002946)

[(2‑8) 7](#_Toc333002947)

[(2‑9) 7](#_Toc333002948)

[(2‑10) 7](#_Toc333002949)

[(2‑11) 7](#_Toc333002950)

[(2‑12) 8](#_Toc333002951)

[(2‑13) 8](#_Toc333002952)

[(2‑14) 9](#_Toc333002953)

[(2‑15) 9](#_Toc333002954)

[(2‑16) 9](#_Toc333002955)

[(2‑17) 9](#_Toc333002956)

[(2‑18) 10](#_Toc333002957)

[(2‑19) 10](#_Toc333002958)

[(2‑20) 10](#_Toc333002959)

[(2‑21) 10](#_Toc333002960)

[(2‑22) 10](#_Toc333002961)

[(2‑23) 11](#_Toc333002962)

[(2‑24) 11](#_Toc333002963)

[(2‑25) 11](#_Toc333002964)

[(2‑26) 11](#_Toc333002965)

[(2‑27) 12](#_Toc333002966)

[(2‑28) 12](#_Toc333002967)

[(2‑29) 13](#_Toc333002968)

[(2‑30) 13](#_Toc333002969)

[(2‑31) 13](#_Toc333002970)

[(2‑32) 14](#_Toc333002971)

[(2‑33) 14](#_Toc333002972)

[(2‑34) 14](#_Toc333002973)

[(2‑35) 15](#_Toc333002974)

[(2‑36) 15](#_Toc333002975)

[(2‑37) 16](#_Toc333002976)

[(2‑38) 16](#_Toc333002977)

LIST OF ABBREVIATIONS

|  |  |
| --- | --- |
| API  CU  GAE  GUI  GWT  FDD  IDE  JDK  JDO  JPA  JVM  MVP  ODE  PaaS | Application Programming Interface  Cranfield University  Google App Engine  Graphical User Interface  Google Web Toolkit  Feature Driven Development  Integrated Development Environment  Java Development Kit  Java Data Objects  Java Persistence API  Java Virtual Machine  Model View Presenter  Ordinary differential equation  Platform as a Service |
| RPC  SDK  SWT  TDD  UI  UT | Remote Procedure Call  Software Development Kit  Standard Widget Toolkit  Test Driven Development  User Interface  Unit Test |
|  |  |
|  |  |
|  |  |

# 1. Introduction

The Introduction chapter focuses on descriptive background to the work and points aims and objectives of the thesis project. All requirements of the project are explained in this chapter. Moreover, main motivators to perform this specific topic are included as well. This chapter also contains literature review, and thesis structure.

## Overview

A series of simultaneously ordinary differential equations model physical systems that evolve over time. There is a wide variety of software available for solving ODE’s. However, it is hard to find an easy to use robust application providing good quality solutions with clear visualisation of the results. This thesis project aims to combine the most efficient and accurate numerical methods, solving ODE’s and systems of ODE’s, with robust web technologies providing modern solution visualisation . There are scientific and technological challenges present in this project. Furthermore, since main part of the thesis is about developing a specific application, issues concerning software development process are also significant.

## Aims and objectives

The main objective of this thesis project is to develop application :

1. Parsing ODE’s and systems of ODE’s entered by the user
2. Solving series of 1st order simultaneous ordinary differential equations (linear or non-linear) for initial value problem, given along with user defined step and domain.
3. Presenting the solution as a 2D graph.
4. Storing and loading equations along with parameters entered by the user.

## Motivation

In general, two main motivators of this project are :

1. Discovering most efficient numerical methods for solving series of ordinary differential equations.
2. Familiarise with AJAX applications development and Google AppEngine along with Datastore.

## Literature review

The literature review gives an insight into the numerical methods solving ODE’s, technologies like Google AppEngine along with Datastore and AJAX – based applications development with emphasis on GWT.

The three major types of practical numerical methods for solving ODE’s [16], [19] are :

* Runge-Kutta methods
* Methods using Richardson extrapolation, especially Bulirsch-Stoer method.
* Predictor-corrector methods (also known as multistep methods)

An extensive study of GWT and AJAX approach [4], [5], [10], [15], [20] noted that utilization of Google Web Toolkit is a good way to achieve robust web application.

Usage of Google App Engine, which is Google’s PaaS, to run web applications is noted to be very good idea in terms of reliability, scalability and robustness [15]. Furthermore, availability of App Engine’s Datastore is described as well integrated and reliable storage [8], [9] .

In terms of software lifecycle models , the Prototyping Model seems the most suitable for this project [2] . From the Agile approach flavours , TDD and FDT are suitable to a certain degree for this thesis [1], [3], [17], [18], [23].

Design decisions were made basing on articles from Google Developers page, containing detailed descriptions of applications development using Google technologies. [11], [13], [14], Moreover, design patterns and architectural details of Google Web Toolkit were taken into account during for better understating of those technologies. [6], [7], [21], [22].

The testing methodology applied for GWT applications is based on Unit Testing and cross-browser UI testing [12], [23].

## Thesis structure

The structure of further chapters of this thesis report are stated below:

* In chapter 2 the mathematical background to the methods implemented in the application is presented
* Chapter 3 contains descriptions of the technologies, methodologies and application design along with software lifecycle model.
* Chapter 4 concerns testing strategies and methodologies undertaken to verify and validate the developed software.
* In chapter 5 the implementation details of the application are presented.
* Chapter 6 is about results achieved in this thesis project
* Discussions and conclusions of the project are presented in chapter 7.

# Mathematical background

This chapter demonstrates knowledge about recommended practical numerical methods for solving ODEs. Presented literature review gives an insight into major types of numerical routines taking into account efficiency and accuracy.

## Ordinary differential equations

An ordinary differential equation is an equation that contains function of one independent variable and its derivatives. General definition of the order :

|  |  |
| --- | --- |
|  | (2‑) |

Important issues involving ODEs are boundary conditions. In other words algebraic conditions on the values of the function . In general they divide into two broad categories [19] :

* Initial value problems

All are given at some starting point and it is desired to find the at some final point or list of points with specified intervals, for example .

* Two-point boundary value problems

Where boundary conditions are specified at more than one point. For example at starting and final point.

General definition of the system of ODEs of order :

|  |  |
| --- | --- |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

## Euler’s method

Euler’s method is a first-order numerical method for solving ODEs . It is not recommended method for practical use, however it is important conceptually for advanced methods .

|  |  |
| --- | --- |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

## ODE numerical routines

This section describes types of practical numerical methods for solving ODEs including Runge-Kutta methods, Bulirsch-Stoer, Rosenbrock methods and Predictor-corrector methods.

### Runge-Kutta methods

Runge-Kutta methods propagate a solution over an interval by combining the data from several Euler-style steps. Each step involves one evaluation of the right-hand of the function .

|  |  |
| --- | --- |
|  | (‑) |

Thenusing the information obtained to match a Taylor series expansion up to higher order.

Developing higher order methods made Runge-Kutta competitive with the other numerical methods in many cases. It is usually the fastest method when moderate accuracy is required (≤ ) and evaluation of the function is not too expensive. There are few kinds of Runge-Kutta methods : 2nd order method, (called midpoint method), 4th order method and also method with adaptive stepsize. [19]

#### 4th Order Runge-Kutta

The most often used Runge-Kutta method is the fourth order formula. In general it is superior to 2nd order method, however high order does not always mean high accuracy. The 4th order method requires four evaluations of the function. [19]

|  |  |
| --- | --- |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |



Figure ‑ 4th Order Runge-Kutta method

During a single step, the derivative is evaluated four times. Once at the initial point, (1) twice at the midpoints (2)(3) and once at the trial endpoint (4). The final function value is calculated on the basis of these derivatives. [19]

Each step in the sequence of steps is treated in an identical manner, so prior behaviour of the solution is not used in its propagation. Such approach is mathematically proper, since any point along the trajectory of an ODE can be an initial point. [19]

#### Runge-Kutta for a system of differential equations

The algorithm of 4th order Runge-Kutta method for solving systems of ODE’s comprises of the following steps :

|  |  |
| --- | --- |
|  | (‑) |

|  |  |
| --- | --- |
| , , … | (‑) |

|  |  |
| --- | --- |
| , … | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

#### Runge-Kutta with adaptive stepsize

The purpose of the adaptive stepsize method is to achieve predetermined accuracy in the solution with minimum computational effort. It is possible to face very smooth interval while performing Runge-Kutta steps. Taking a few great strides instead of small steps should speed through such undifferentiated interval, what may result in significant gain in efficiency. The idea of the adaptive stepsize method is to control the size of the step and increase it when possible maintaining the required level of accuracy. It is important to estimate the truncation error to control the accuracy level while increasing the step size. Obviously the calculation of this information will add to the computational overhead, however it is a profitable investment in terms of efficiency. [19]

### The modified midpoint

The modified midpoint method is a second order method like 2nd order Runge-Kutta, however with the advantage of requiring only one derivative evaluation per single step instead of two evaluations present in Runge-Kutta. This method generates the solution as a vector of values from a point  to a point by a sequence of substeps each of size . [19] Where

|  |  |
| --- | --- |
|  | (‑) |

The total number of function evaluations required by this method is . The formulas essential to provide the solution for are as follows

|  |  |
| --- | --- |
|  | (‑) |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

The is the final approximation to whereas represents intermediate approximations calculated along in steps of .

#### Modified midpoint for a system of differential equations

The form of the Modified midpoint method for solving system of ODE’s is presented below

|  |  |
| --- | --- |
|  | (‑) |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

|  |  |
| --- | --- |
|  | (‑) |

### Richardson extrapolation

Richardson extrapolation bases on idea of extrapolating a computed value to the value that would have been obtained if the stepsize had been remarkably smaller than it actually was. The practical numerical method using this idea is called Bulirsch-Stoer method.

#### Bulirsch – Stoer

The idea of Burlisch-Stoer method is to perform iterations of the modified midpoint method. Each iteration uses various number of substepsfor the modified midpoint method and ends up with polynomial extrapolation of the given values. [16], [19] Burlish and Stoer originally proposed the following sequence of substeps :

|  |  |
| --- | --- |
|  | (‑) |

However the sequence discovered by Deuflhard is usually more efficient :

|  |  |
| --- | --- |
|  | (‑) |

In terms of number of iterations usually 8 gives satisfactory results.



Figure ‑ Richardson extrapolation used in the Burlisch-Stoer method with substep n = 2,4,6 [19]

We use Aitkens-Neville algorithm in order to perform extrapolation, which is described by the following tableau :



Figure ‑ Aitkens-Neville polynomial extrapolation tableau [19]

The first column of the tableau is formed by modified midpoint first iteration with n = 2 .

|  |  |
| --- | --- |
|  | (‑) |

Where is computed with the stepsize

Successive columns can be filled by using following recurrence :

|  |  |
| --- | --- |
|  | (‑) |

The final solution which is can be achieved after performing each successive iteration [16]

### Rosenbrock

Rosenbrock methods are competitive with other numerical ODEs integrators in terms of moderate accuracies (tolerances of order . Moreover these methods remain reliable for more stringent parameters [19] . The main formula of the Rosenbrock method is as follows :

|  |  |
| --- | --- |
|  | (‑) |

Where corrections are found after solving following linear equations :

|  |  |
| --- | --- |
|  | (‑) |

The coefficients are fixed and Jacobian matrix is denoted by . [19]

### Predictor- Corrector

Predictor – Corrector methods are a subcategory of methods called “multistep” and “multivalue”. These methods have had long historical run. It is said that that predictor-corrector integrators have had their day. For high precision applications and right-hand side expensive evaluations Bulirsch-Stoer method dominates. For moderate precision problems Runge-Kutta methods dominates. However there is possibly one exceptional case where predictor-corrector dominates. It is the case of high-precision solutions of very smooth equations with complicated right-hand side evaluations [19].

Considering the multistep approach it is important to realize the difference between integrating an ODE and finding the integral of a function. For a function, the integrand has a dependence on the independent variable . However for an ODE, the “integrand” (which is right-hand side) depends both on and dependent variables [19]. So in order to advance the solution of from to we have :

|  |  |
| --- | --- |
|  | (‑) |

According to a multistep approach is approximated by a polynomial passing through several previous points and possibly through .

The formula that is evaluating the integral (2-18) at is then of the form:

|  |  |
| --- | --- |
|  | (‑) |

where

There is a method called which solves an implicit formula of the form (2-19) for . Such method is called a . The idea of this method is to take initial guess for , then insert it into the right-hand side of (2-19) and get updated value of . In order to get initial value of we have to extrapolate the polynomial fit to the derivative from the previous points to the new point . The next stage of solving process is made by which is using the prediction step’s value of to the derivative [19]. In conclusion Predictor-corrector method comprises of three separated processes :

* Predictor step
* Evaluation of the derivative from the latest value of .
* Corrector step

#### Adams-Bashforth-Moulton

Probably the most popular method is method. This method has good stability properties [19] . The predictor part is called The Adams-Bashforth :

|  |  |
| --- | --- |
|  | (‑) |

The Adams-Moulton part is the corrector :

|  |  |
| --- | --- |
|  | (‑) |

In order to perform this method it is necessary to evaluate and having initial value ( . To achieve this you have to use other numerical routine to evaluate two steps. Usually 4th Order Runge-Kutta method is used for this.

For systems of ordinary differential equations, predictor and corrector steps are transformed into following equations :

Predictors :

|  |  |
| --- | --- |
| … | (‑) |

Correctors :

|  |  |
| --- | --- |
| … | (‑) |

# Technologies, Methodologies and Application Design

This section is a combination of methodologies chosen for this thesis project and design part. The chapter presented here includes description of software lifecycle model which was chosen for this project. Moreover, a description of the agile approach applied in this thesis is also given. The AJAX approach is taken into account along with Google Web Toolkit. Also Google App Engine’s possibilities for maintaining web-based applications are described.

## AJAX approach

AJAX which stands for Asynchronous JavaScript and XML refers to a set of web-development techniques including the use of JavaScript, CSS and asynchronous HTML requests. The biggest advantage of this set of techniques is bringing desktop-like experience to the client-side of a web application. AJAX applications asynchronously request only the necessary information from a server. That is why they reduce the traffic and the server load comparing to non-AJAX web applications , which synchronously request whole web pages from their servers. Good example to realize it is following situation. Users are trying to log in to their e-mail application. After authentication process the only real job of the application is to replace a login link by some user welcoming message. Following figure presents how web traffic is happening for AJAX and a HTML-only non-AJAX applications for described scenario. [4], [5], [15]



Figure ‑ Comparison of AJAX light traffic needs versus legacy HTML applications [15]

## Technologies used

Part of literature review concerning technologies helped with making decisions about which technologies, tools and frameworks to use. The project is designed as an AJAX application using **Google Web Toolkit 2.4** .

**Google App Engine** (SDK version 1.6.4) is responsible for running application and storing data on the Datastore. It is also responsible for automatic scaling and load balancing [4], [5], [15].

**Objectify** as an lightweight and effective framework is used to simplify working with Datastore.

**Exp4j** library is applied in ODE Solvers implementation. It is capable of evaluating expressions and functions in the real domain . This library is very useful for evaluation of right-hand-side functions in numerical routines implemented in the ODE Solvers.

In order to provide good quality 2D chart presenting solution , **Google Chart Tools 1.1** library is used. It is also called and provides wide variety of charts and graphs.

In order to provide rich GUI , **Ext GWT** (**GXT) 2.2.5** library was used. It is a Java library for building internet application with GWT.

### Google Web Toolkit

Google Web Toolkit is a development toolkit that enables you to build AJAX applications using the Java language which is compiled to JavaScript. GWT minimizes the cross-browser issues and enables productive development of high-performance web applications. It encapsulates the object API and provides a set of ready-to use interface components and widgets. Google Web Toolkit provides framework for building RPC services, which provide certain functionalities that can be accessed asynchronously from web application [4], [5], [15].



Figure ‑ An overview of GWT approach

GWT consists of four main components listed below, which provide functionalities for writing AJAX applications [4], [5], [15].

* **GWT Java to JavaScript Compiler**

GWT compiler compiles and optimizes GWT applications written in Java to JavaScript. That is why an application can be deployed to a web container.

* **GWT Hosted Web Browser**

This component enables you to run and execute GWT applications in JVM , in hosted mode, without compiling to JavaScript . GWT provides such possibility by embedding a special SWT browser control, that contains hooks into the JVM.

* **JRE emulation library**

Contains JavaScript implementations (for the client-side implementation ) of most widely used packages in Java standard class library like , which are used on the client-side. On server-side implementation you are free to use entire Java class library.

* **GWT Web UI class library**

This provides a set of interfaces and classes that enable you to create various UI components and widgets. Moreover you are free to use ready-to-use widgets in your applications.

#### GWT Remote Procedure Calls

In GWT, client-server communication is enabled using mechanism. Each side of the process implements GWT service interface for sending and receiving special GWT serialized data. The server side exposes resources and client side invokes those resources asynchronously [5].

### Google AppEngine

Google App Engine is a PaaS cloud computing platform for developing and hosting web applications using Google’s servers and infrastructure. Supports Java, Python and Go runtime environments. GAE as a platform is designed for scalability , robustness and performance. It is very well integrated with Google Web Toolkit. Once you develop application using GWT, you can deploy it on the GAE [15].

App Engine distributes requests for applications across multiple web servers to prevent application from interfering with another. In order to achieve it applications run in a restricted “sandbox” environment. Applications in this environment can execute code, store and load data from App Engine’s Datastore and examine web requests [15].

In terms of limitations , an App Engine application cannot :

* Write to the filesystem. All operations connected with storing and quering data have to be done using Datastore.
* Access another host directly or open a socket.
* Make some other kind of system call

### Datastore

The Google App Engine’s Datastore is a non-centralized persistent store, based on Google’s BigTable technology. It provides robust and scalable storage for web applications running on App Engine. Datastore is not a relational database based on join queries, it is rather a property-value store holding specified objects known as . It was designed to manage scaling to very large data sets in distributed architecture. For this reason Datastore is different than traditional relational databases [8].

Java Datastore API provides low-level operations on entities. Google App Engine SDK includes implementations of JDO and JPA interfaces for modelling and persisting data. It is possible to use Datastore API directly in your applications, however there is also an option to use a framework which simplifies Datastore usage for Java developers. There are three frameworks recommended by Google App Engine team [8], [9].

* **Objectify**

Very simple and convenient interface to the App Engine Datastore. Helps with avoiding some complexities of JDO/JPA and low-level Datastore.

* **Twig**

This framework provides a configurable object persistence interface that improves support for inheritance, polymorphism and generic types. Similarly to Objectify helps you to avoid Datastore complexities.

* **Slim3**

Slim3 is not limited only to Datastore. It is a MVC framework which can be used for wide variety of App Engine functions.

As mentioned at the beginning of this chapter, framework chosen for this project is .

Each has one or more named properties . Each property can have one or more values. The available data types defined for Datastore are presented in Appendix A.

There are following limitations concerning Datastore :

Table ‑ Datastore limitations

|  |  |
| --- | --- |
| Limit | Amount |
| Maximum entity size | 1 megabyte |
| Maximum transaction size | 10 megabytes |
| Maximum number of values in all indexes for an entity | 5000 |
| Text string (short) | Up to 500 Unicode characters |
| Text string (long) | Up to 1 megabyte |
| Byte string (short) | Up to 500 bytes |
| Byte string (long) | Up to 1 megabyte |
| Floating-point types | 64-bit double precision |

### App Engine Administration console

Google AppEngine provides Administration console for every AppEngine’s account. It is very useful for managing and monitoring deployed applications. Moreover it is possible to provide basic configurations, set performance options and manage versions of deployed applications. Furthermore Datastore configuration options are also available there. An example of such console view is available in Appendix B.

## Architecture

From the very beginning of this thesis, the idea was to develop it as a web application. The main reason is to make it accessible from any web browser and ready to use without installation. The application is divided on the server-side and client-side implementation.

The application is divided into several modules :

* **Equation Parser**

This module is responsible for parsing user’s input into ODE objects or System of ODEs objects .

* **ODE Solver**

Contains implementations of ODE numerical routines. The Solver operates on objects returned by the Equation Parser.

* **Graph Viewer**

This component is responsible for presenting Solution object, returned by the ODE Solver, as a 2D graph with intervals specified by the user.

* **Equation store**

This module is a Datastore connector, which is responsible for storing and quering Equations on the Datastore.



Figure ‑ Application architecture overview

According to good software design and development practices, Equation Parser, Equation Store and ODE Solver are processed on the server-side of the application. The client-side implementation contains User Interface and Graph viewer.

## Design patterns

The whole structure of the application is kept in MVC pattern to maintain separation of concerns.

Command and Composite are design patterns used in GWT.

The Command pattern encapsulates a request as an object. In fact this pattern lets toolkit turn the request itself into an object, which can be stored and passed around like other objects. In other words Command objects can be thought of as “tokens” that are created by one client that knows what need to be done and passed to another client that has required resources to perform this operation.



Figure ‑ Example of Command Pattern structure [21]

Composite is a structural pattern, which composes objects into tree structure to represent whole-part hierarchies. The idea of this pattern is to compose objects in such a way that client sees many of them as single objects. The advantage of applying Composite pattern is using some operations for an object in the same way as for group of objects.



Figure ‑ Example of Composite Pattern structure [22]

## The Prototyping Model

The prototyping lifecycle model is an example of an Evolutionary model. In general prototype means a version of the software used to test different solutions to the problem. Such approach allows better understanding of the ways solution might work and could be useful to choose the best solution for the final version of the software. The most important factor in prototyping is the feeding back of experience from each iteration into improving the design [2] .



Figure ‑ The prototyping lifecycle

During development process of this thesis project, features of the application were developed according to the prototyping model. At the beginning of the cycle, requirements are gathered. Then a quick design phase is performed. Another step is to develop a prototype according to the prepared design. The next step is evaluation of the developed prototype in agreement with thesis supervisor. Another step is gathering comments about prepared prototype and refining it by repeating the cycle from design part. This process is repeated as long as feature requires improvements and corrections .

## Agile approach

The key ideas of Agile approach are reacting on changes in project quickly and loose grouping of similar software process models. In other words, developing model sets up lightweight structure of the project with practical hands-on approach and intensive usage of evolutionary and iterative methods. Moreover, in this approach customer plays an active part in a development process.

### Feature Driven Development

FDD is an agile approach which treats project as a set of features and can be used on almost any project regardless of size and technology.

The first process in FDD is to develop overall model of an application. The idea of this stage is to gain good understanding of the problem domain.

The second process is to prepare a list of features. Each feature is a small client-valued requirement which typically takes 1-3 days to implement.

The third and last process is called “Plan by Feature” . Taking into account risks and dependencies of the features, the order of the features to develop is prepared. [17]

### Test Driven Development

Test Driven Development is also one of the Agile methodologies used in this project. In traditional testing approach tests are created after developing some piece of software. TDD turns traditional approach around. Instead of writing functional code first and then testing code as an afterthought , you write test code before functional code. Furthermore, the best way to perform TDD is by making small steps, one test and one small bit of corresponding functional code. It sounds simple in principle, however requires great discipline. It is easy to “slip” and write functional code avoiding new tests. [1], [2]



Figure ‑ Test Driven Development cycle

## Software versioning

In terms of software versioning and revision control, whole development process was supported by Google Project Hosting, which provides fast, reliable and open source hosting service. The IDE was used to develop the software and plugin was supporting Subversion system within this IDE.

# Testing

Testing is an important part in a software development process. In terms of GWT applications, the testing infrastructure is based on classes.

## Unit testing

This represents the lowest level of testing in validation and verification process. The aim of single UT is to check correctness of the smallest component of source code, usually a method of a class.[3]

### GWT Unit Testing infrastructure

Since a GWT application is written in Java, you are free to use JUnit as a Unit Testing framework. Google Web Toolkit provides which is a subclass of JUnit’s . This class is necessary to test native JavaScript code. Such UT can be performed on hosted-mode browser, provided by GWT. In fact there is no difference for a developer between using standard class and class, only is an additional method which must be implemented. This method returns a string containing the name of GWT code module as defined in module configuration file of the application. Running test cases extending starts up hosted-mode browser and then evaluates prepared tests against it. Such testing infrastructure allows invoking asynchronous RPC calls, run native JavaScript functions and render widgets. [23]

### TDD approach

The TDD approach is used in this thesis project to a small extent. The vast majority of unit tests prepared for ODE Solvers was written before implementation phase. The idea was to define set of specific ODEs checking correctness of the solvers. [1]

### Test Cases

There are several Test Cases prepared to verify correctness of the developed software :

#### ParserTestCase

Contains tests concerning Equation Parser component. There is a wide variety of tests checking parser reactions for a correct and incorrect input as well.

Table ‑ Parser Test Case : correct ODE’s

|  |  |
| --- | --- |
| Test name | Parser input |
| testCorrectEquation1 | y' = y + x, y = 0 |
| testCorrectEquation2 | y''' = y + x, y=0 |
| testCorrectEquation3 | y ' ' ' = y+x, y = 0 |
| testCorrectEquation4 | y''' = y'' + y' + y + x = 5, y = 0 |
| testCorrectEquationFunction | y''' = y '' + y\*y' - y + x + 4, y = 0 |

Set of tests checking parser for correct ODE’s. Presented tests differs from each other in terms of equation’s complexity and order.

Table ‑ Parser Test Case : incorrect ODE’s

|  |  |
| --- | --- |
| Test name | Parser input |
| testNoODE | y + x |
| testNoODEWithInitVariable | y = tre , y = 0 |

Tests performed within this Test Case provide characters put together which are not constituting a differential equation.

Table ‑ Parser Test Case : equation’s incorrect variables

|  |  |
| --- | --- |
| Test name | Parser input |
| testToManyVariables | y’ = y + x + z, y = 0 |
| testNoIndependentVariable | y''' = y '' + y\*y' - y + 4, y = 0 |
| testTooManyIndependentVariables | y''' = y '' + y\*y' - y + 4 + x + u, y = 0 |

This Test Case verifies parsing ODE’s containing incorrect and correct states of variables in an equation. There are tests performed containing too many variables in an equation. Moreover an equation which has no independent variables is verified in terms of correctness for the parser.

Table ‑ Parser Test Case : case sensitivity

|  |  |
| --- | --- |
| Test name | Parser input |
| testCaseInsensitivity | y'' = y + x + 2\*X + 3/Y', y = 0 |

This test checks whether equation is correctly parsed when characters are case insensitive.

Table ‑ Parser Test Case part 7

|  |  |
| --- | --- |
| Test name | Parser input |
| testMathExpressions | y'=sin(x)+cos(x)+exp(x)+log(x)+tan(x)+sqrt(x), y = 0 |

Test verifies if mathematical expression are supported by the parser.

Table ‑ Parser Test Case : initial values

|  |  |
| --- | --- |
| Test name | Parser input |
| testWrongInitVariable | y' = y +3, u =4 |
| testNoInitVariable | y' = x + 4 |

This Test Case is verifying if exception is being thrown when initial values of the equations are omitted. Additionally another test is performed to check situation when initial values concern irrelevant variables.

Table ‑ Parser Test Case : system of ODE's

|  |  |
| --- | --- |
| Test name | Parser input |
| testSystemOfODE | "y'= y + x, y = 0" ,  "z'= z + y + x, z = 0" |

The idea of this test is to verify parsing systems of ODE’s.

#### SolverTestCase

The is a base class for all Test Cases prepared to verify the correctness and accuracy of the ODE Solvers implemented. In order to get correct solutions, which are essential for comparison in unit tests, system was used. It is using an online mathematical system called , which is very precise and efficient when it comes to ODEs solving. All ODE Solver Test Cases extend and perform the same tests. The only difference is an error tolerance, which depends on the method implemented. Every class implements :

**public** **void** gwtSetUp()

Which contains specific Solver’s initialization and accuracy setting.

In terms of , it comprises of the following tests :

Table ‑ Solver Test Case : 1st order linear ODE

|  |  |
| --- | --- |
| Test name | Equation content |
| test1OrderEquation | y'=-2\*y+x+4 |

Tests verifies result of the Solver within a range [0.0 , 0.2] and step = 0.01 for the linear ODE. The correct answer was provided from analytic solution of the ODE. Tests checks number of solution values included in object and value at the point 0.2.

Table ‑ Solver Test Case : 1st order non-linear ODE

|  |  |
| --- | --- |
| Test name | Equation content |
| test1OrderMathPowerEquation | y'=y+x^2 |
| test1OrderMathSinCosEquation | y'=sin(x)+cos(x) |

This set of tests verifies accuracy of non-linear ODE’s. Both tests are performed with the domain [0.0 , 1.0] and step 0.1. Solution compared in these unit tests is achieved using ‘s .

Table ‑ Solver Test Case : 1st order system of ODE's

|  |  |
| --- | --- |
| Test name | System of ODE’s |
| test1OrderSystem | y'= y + x  z'= z + y + x |
| test1OrderSystem3 | y'= y + x  z'= z + y + x  u'= u + x + 4 |

Tests provided in this Test Case verify solution accuracy for systems of ordinary differential equations. The and check accuracy of a system which comprises of respectively two and three ODE’s. The domain for all equations is defined as [0.0 , 1.0] with step = 0.1 . All initial values for the functions , and (in the second system) are 0.0 .

## Black-Box testing

The idea of black-box testing is to test software according to requirements specification, without any knowledge of internal structure. According to this approach application is treated as a “black-box” and testing process is basically based on performing use cases of the application.

Since vast majority of use cases can be covered with unit tests for this project, black – box tests concern user interface tests mainly.

Functionalities of the application were tested according to black-box testing strategy on different web browsers :

* Google Chrome 20.0
* Mozilla Firefox 14.0.1
* Microsoft Internet Explorer 8.0

### Persistence tests

This set of tests is responsible for testing component. Tests performed are checking operations of storing and querying data on Datastore. There is a reason why these tests are not performed as a separated TestCase comprising of unit tests. It is possible to perform local testing of Datastore by using class from library. However those tests can be performed on Datastore interface only. It means that it is not possible to perform implemented services using Datastore and objectify locally. This is the reason why module is tested using black-box methodology. Several tests are performed to cover all possible scenarios related to Datastore usage as stated below :

* store an equation
* load an equation
* store system of equations
* load system of equations
* list all systems of equations
* remove system of equations
* remove all systems of equations

# Implementation

This Implementation chapter is divided into four parts according to main application’s modules . As mentioned before, the implementation is organised according to MVC pattern. Furthermore, the structure of the project is kept as a typical GWT application structure.

## The anatomy of the project

This project is structured according to the GWT application convention. The most important parts of project are as follows :

* **client package**

This package contains client-side implementation. This code will be cross-compiled to JavaScript. Includes

* **server package**

Server-side implementation, contains Equation Parser, ODE Solvers and Persistence services.

* **shared package**

This package contains all classes used on server-side and client-side implementation. It includes and packages, which contain classes used in both implementations.

* **ThesisAE.gwt.xml**

GWT module definition file. Declares several primary elements : inherited modules, servlet deployments, compiler plugins and entry points.

* **web.xml**

Contains mappings for servlets specified in the .

* **ThesisAE.java**

Main class of the application, implements . It is the starting class invoked by the module.

## Model

According to MVC pattern which is used in this project there is separated model implementation located in package. That is why all model classes are available for client-side and server-side implementation. Model comprises of the following classes:

### Equation

It is a very important class, which represents equation in the application. Equation is created after parsing stage, and ODE solvers are operating on it during solving process. This class representation is based on following data :

**private** List<Double> initValues;

**private** String equationContent;

**private** **char** independentVariable;

**private** **char** functionVariable;

**private** **int** order;

initValues stores equation’s initial values, equationContent is a content of the equation presented as a string, independentVariable and functionVariable are represented as characters and order is an order of the equation stored as int.

All class methods are standard data accessors, which for Java programming language are so called setters and getters. Moreover several constructors were implemented to instantiate an object depending on the data available to create such an object.

### System

The System class represents system of equations in the application, which are stored in a list :

**private** List<Equation> equations

Except standard setters and getters, the class provides :

**public** **void** addEquation(Equation equation)

which enables scenario when you creates object and adds equations one by one.

### SystemEntity

This class is an entity class represented in AppEngine’s Datastore. It is an expanded version of the in terms of information stored as stated below :

@Id

**private** String name;

**private** List<String> equations;

**private** **double** min;

**private** **double** max;

**private** **double** step;

**private** Date date;

Except the list of equations there is, inter alia, name variable, which is an entity’s identifier in a Datastore. Furthermore, min and max indicates the borders of the interval and step represents a step which a system will be solved with. Finally there is date which stores the date when was last modified on the Datastore.

This class is also used to store single objects in Datastore. Such entity simply contains only one in the list.

### Solution

The class is a representation of the result provided by the ODE Solver. The structure of the data represented by this class is following :

**private** List<Double> results

**private** **double** min

**private** **double** max

**private** **double** step

List of the values provided by the solver is stored in results. Other variables min, max and step are necessary for presenting a solution on the graph.

## Equation Parser

Equation Parser is implemented as the service. This class includes set of methods necessary to perform parsing operations on user input.

### ParserServiceImpl

**public** Equation parseEquation(String input) **throws** IncorrectODEEquationException

The main method responsible for parsing ODE, given parameter is a input provided by the user. Method returns object which includes all equation data necessary for the ODE Solver.

There are several steps to the parsing process. At the beginning, input is separated into equation content and initial values part. Then following methods of are executed to finish the process :



Parses initial values



Retrieves character which stands for a function in parsed equation.

Retrieves character which stands for an independent variable of the function in the equation.

**public** System parseEquationsSystem(List<String> inputs) **throws** IncorrectODEEquationException

This method is responsible for parsing the System of Equations, the parameter is a list of equations in a form provided by the user. As a result the method returns a object including data necessary for the Solver module.

Parsing a system of equations seems like performing a loop of equation parsing, however the process of evaluating independent and functional variables of the system has to be done regarding all equations. It means that and methods are performed respectively for all equations, but the overloaded method is executed at the end with a list of all equations in a system.

- is the exception which is thrown when some part of equation or system of equations is incorrect during the parsing process. This exception includes message which inform about the reason of the exception.

## ODE Solvers

There are a few important classes which form ODE Solver module.

### Solver base class

This is a base class for all specific numerical methods solving ODE’s. and contains a set of methods which are common for all implemented solvers. Those methods are basically operations on lists and vectors like addition of vectors along with multiplying by some specific .

### ODE Solver services

The 4th order Runge – Kutta method is implemented as . The Modified Midpoint method is implemented as and Predictor-corrector as . All specific solvers extend mentioned class and provide two methods. One for solving ODE’s and second for solving a systems of ODE’s.

**public** Solution solve(Equation equation, **double** step, **double** start, **double** stop) **throws** IncorrectODEEquationException, UnknownFunctionException, UnparsableExpressionException.

This method is responsible for solving ODE given as an parameter. Other parameters : and define domain of the equation. The solving process is controlled by the parameter, which influences the level of accuracy of the solution. The method returns object which contains results.

## Graph Viewer

This module belongs to the client-side implementation. The objective of this component is to provide a graph presenting the solution of the given equation or system of equations. The class which implements inter alia Graph viewer module is . It contains private classes : and which are callbacks for ODE Solver’s methods and respectively. Those private classes set graph properties and values received from ODE Solver as object. Then class from library is created in order to provide visualisation of the 2D graph presenting the solution.

## Equation Store

This module is responsible for data persistence in the application. is a service providing set of methods for storing and querying systems of equations in Datastore. Implementation is based on the Objectify framework which significantly simplifies coding part of this service. provides the following interface :

**public** **void** persist(SystemEntity system)

This method stores system of equations in the Datastore.

**public** SystemEntity get(String name)

Gets system of equations specified by the parameter, since is identified by field.

**public** List<SystemEntity> getAll()

This method provides all stored systems of equations as a list. It is especially useful for presenting available systems to load for the user.

**public** String remove(String name)

This method enables removing from Datastore, specified by parameter.

**public** **void** removeAll()

Removes all stored systems of equations from Datastore.

## User interface

In order to provide rich and robust user interface Ext GWT (GXT) along with standard GWT components were used. GUI comprises of three panels : and .

### Input Panel

This panel comprises of several subpanels. Combined all together create interface for the user to provide, load or save equation or system of equations. Furthermore user defines domain borders, step and chooses one of three implemented methods solving ODE’s . Additionally some sort of help is included in Input Panel. The user can familiarize himself with the format of equations and systems of equations by checking examples. Moreover a list of available mathematical expressions is also provided. Finally, after providing all necessary information the user can press “Compute” button at the bottom of the panel.

In terms of implementation details class extends from Ext GWT library. Vast majority of components, events and listeners in this class is based on GXT library. The structure of subpanels maintained by the from standard GWT library. Moreover, to provide unlimited text fields for the equations was used. This specific table enables creating cells on demand. Such functionality is used to add another text fields when user provides another equations into the input.



Figure ‑ Input Panel

### Equation Panel

The objective of this panel is to present equations after the parsing process. It is important from the user’s point of view to check how the provided input was interpreted.

The implementation of this panel is based on is used to store rows containing parsed equations, which are represented as objects including equations contents. These images with equations are created with charts API, supported by standard GWT library.



Figure ‑ Equation Panel with example of ODE's system

### Graph Panel

This class includes 2D graph utilization, provided by Google Chart Tools 1.1 library. Furthermore, the implementation contains quite a few important inner callback classes which drive the main process of the application. and classes implement mechanism of applying received solutions to the object.

Similarly to previously described panels, uses a mixture of GXT and GWT components and listeners. Additionally, package (Google Chart Tools library) is widely used in terms of 2D graph implementation.



Figure ‑ 2D graph presenting solution of sample system of ODE's

### Equation Store GUI components

All operations connected with and Datastore in general, can be performed by the user with following components of the application.

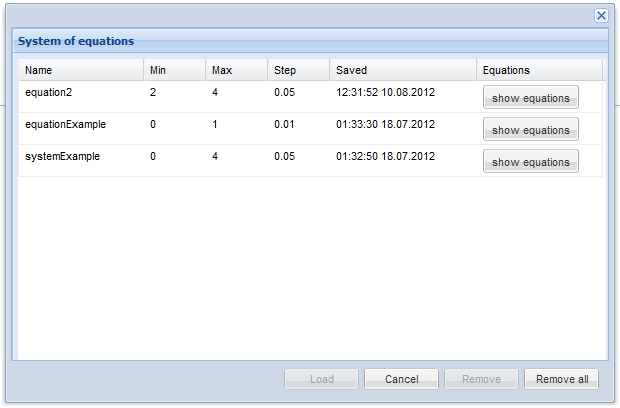


Figure ‑ Developed dialog for loading systems of equations

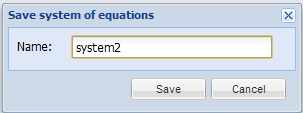


Figure ‑ Developed dialog for saving systems of equations

### Errors handling

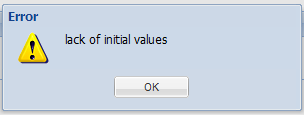


Figure ‑ Example error dialog

# Results

This chapter presents application’s results, with emphasis on Unit testing results. The key part of the project is ODE Solver implementation of numerical methods. However, other components covered with Test Cases are also important in terms of functional requirements of the application.

## Parser Test Case results

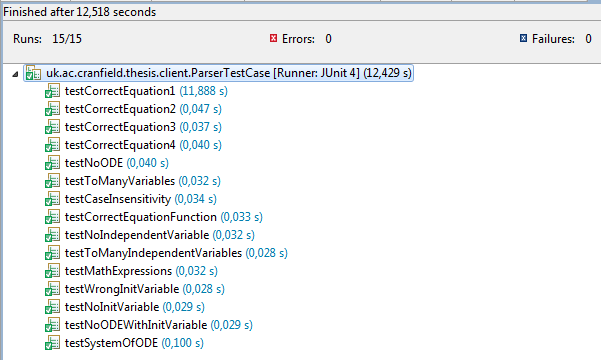


Figure ‑ ParserTestCase results

All unit tests prepared for module passed successfully after many corrections in the software. The vast majority of the tests were prepared according to TDD approach, so before implementation. However, few tests were written at the end of the process to cover scenarios where bugs occurred during black-box testing.

## Solver Test Cases

The results of the tests performed to validate module’s functionality along with verification are presented in this chapter. Furthermore, this section presents the statement of all ODE Solvers implemented, along with accuracy levels and tests passed.

### RungeKuttaSolverTestCase results

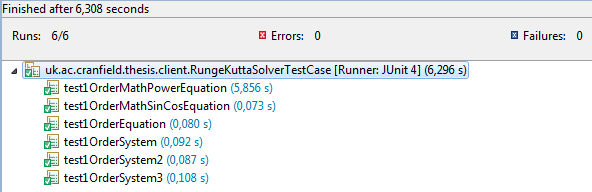


Figure ‑ Runge Kutta TestCase results

The extends . The key point of this class is to perform tests for 4th order Runge-Kutta method. The accuracy is set to . At this level all kinds of tests pass. Moreover, increasing the level of accuracy to causes failure only of one test ( which tests solving linear ODE’s. After accuracy being increased up to all tests prepared for non-linear ODE’s still pass, what is more some of them are still “green” with level of accuracy equals to .

Table ‑ RungeKutta tests results regarding accuracy

|  |  |  |  |
| --- | --- | --- | --- |
| test \ accuracy |  |  |  |
| *test1OrderMathPowerEquation* |  |  |  |
| *test1OrderMathSinCosEquation* |  |  |  |
| *test1OrderEquation* |  |  |  |
| *test1OrderSystem* |  |  |  |
| *test1OrderSystem2* |  |  |  |
| *test1OrderSystem3* |  |  |  |

### ModifiedMidpointSolverTestCase results

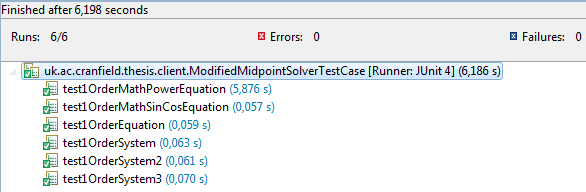


Figure ‑ Modified Midpoint TestCase results

Another TestCase validates and verifies the Modified Midpoint method implemented. It is 2nd order method as mentioned before, so the accuracy is only , however big advantage of this method is performance. The change of accuracy to results in only two tests passed : and . These tests are prepared to verify linear and non-linear ODE’s.

Table ‑ Modified Midpoint tests results regarding accuracy

|  |  |  |  |
| --- | --- | --- | --- |
| test \ accuracy |  |  |  |
| *test1OrderMathPowerEquation* |  |  |  |
| *test1OrderMathSinCosEquation* |  |  |  |
| *test1OrderEquation* |  |  |  |
| *test1OrderSystem* |  |  |  |
| *test1OrderSystem2* |  |  |  |
| *test1OrderSystem3* |  |  |  |

### AdamsBashforthMoultonTestCase results

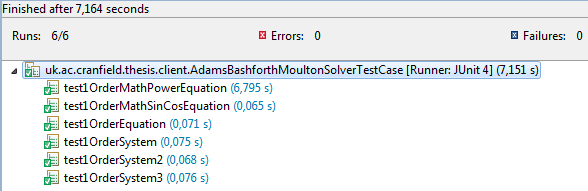


Figure ‑ Adams Bashforth Moulton TestCase results

The accuracy applied for this TestCase is . At this level all tests passed . Moreover, by increasing the level to only failed.

Table ‑ Adams Bashforth Moulton tests results regarding accuracy

|  |  |  |  |
| --- | --- | --- | --- |
| test \ accuracy |  |  |  |
| *test1OrderMathPowerEquation* |  |  |  |
| *test1OrderMathSinCosEquation* |  |  |  |
| *test1OrderEquation* |  |  |  |
| *test1OrderSystem* |  |  |  |
| *test1OrderSystem2* |  |  |  |
| *test1OrderSystem3* |  |  |  |

# Discussion and conclusion

This chapter reviews all stages of the project along with closing remarks and future work ideas.

## Analysis of numerical methods

Facing all reasonable practical numerical routines with requirements for this project, choices about methods to implement were made. The first choice is method. It is a very efficient and accurate method in most cases in terms of ODE’s. Furthermore, it is step driven numerical routine, what fits project requirements.

Another implemented method is . It is very efficient 2nd order method with improved accuracy by intermediate approximations applied. Despite this improvement, this method has some troubles with non-linear equations. Overall accuracy is worse comparing to method, however the advantage is better performance.

The last implemented method is , one of Predictor-Corrector routines. This numerical method is step dependent, what satisfies requirements. It is very efficient method, since only and steps take part in iteration of this routine. This method is still widely used in highly rated available software for solving ODE’s. In terms of accuracy, results are especially good for smooth equations.

The main reason why method was not implemented in this application is performance. This routine based on Richardson extrapolation is very efficient and accurate in terms of devising solution at some specific point. However, it is not possible to use previous evaluation to perform another step. It means that in step driven ODE Solver the only way to apply this method is to perform the whole routine for each step separately. Such a solution requires too many evaluations, especially for tasks with significant number of steps.

methods were found to be computationally complex offering only moderate accuracies. In general this type of methods is less efficient than competitors because of plenty matrix multiplications involved in ODE solving process.

## Analysis of application’s architecture

Suggested architecture for scalable GWT applications is Model View Presenter. This design pattern decouples application into following components :

* Model
* View
* Presenter
* AppController

The presented architecture is very similar to MVC. The Presenter contains all the application’s logic and AppController handles logic that is not specific to any presenter and instead resides at the application layer. The key element in this architecture is which is responsible for passing and registering events in the application.

The described architecture is a very good choice for large scale applications receiving plenty of events. However it is not necessary for GWT applications which uses limited number of events to always follow MVP pattern. In exchange good separation of responsibilities can be provided using MVC pattern. When the number of possible event types is relatively small, there is no danger of turning into messy code having good separation of concerns. So usage of is not always worth it in terms of GWT applications development.

The decision was made to develop this thesis project according to MVC since this specific application will not operate on big amounts of events. On the other hand change of architecture from MVC into MVP is not impossible for GWT applications. After extending application in terms of new features, what will probably increase number of events, MVP pattern is worth considering.

## Results analysis

The level of correctness of the implemented ODE solvers can be estimated by the level of the accuracy set for Test Cases. Tables 6.1, 6.2 and 6.3 present results of ODE Solvers in terms of accuracy.

It is clearly visible that 4th Order Runge-Kutta method provides the best accuracy among all implemented methods. All tests passed with accuracy level set to . Moreover, only one test failed after accuracy increased to . The last column at the Table 6.1 shows that even at level of this method provides correct results for non-linear ODE’s.

The second implemented numerical routine is the Modified Midpoint method. The 2nd order of this method reflects lower level of accuracy. However this method is the most efficient among all implemented ones. All tests dedicated to this method passed with accuracy set to . The level of results positive only with linear and non-linear ODE tests. Finally , increasing accuracy to ended up with only linear ODE test passed.

The Adams-Bashforth-Moulton method provides compromise of efficiency and accuracy among implemented methods. All tests run for this method passed with accuracy set to . After increasing the level to only one test for non-linear ODE failed, what shows very good accuracy results comparing to 4th order Runge-Kutta method. However the final increase of accuracy to resulted in failure of all tests. It shows that this method is accurate to some limit.

## Problems faced

Apart from minor problems related to design, implementation and testing process there was a situation which took more time to solve than other issues. The problem was with Java version incompatibility between App Engine and the developed application. Initially the project was developed using Java 1.7 version. At the moment of writing this thesis, App Engine (SDK version 1.6.4) supports Java 1.6 runtime environment. Running application using some Java 1.7 features on GAE caused a lot of bizarre errors and exceptions. After significant research of this topic, issue was solved. The only possible way was to develop thesis project using JDK 1.6 . However it took some time to identify the source of the problem.

## Conclusion

According to the aims and objectives included in the chapter 1.4, a summary of work carried out is stated below :

1. Equation Parser module implements equations and systems parsing functionality.
2. ODE Solver module implements three selected numerical routines solving series of 1st order simultaneous ordinary differential equations (linear or non-linear) for initial value problem. User can provide domain’s range and step through easy to use GUI.
3. Graph Viewer module implements visualisation of the solution as a 2D graph.
4. Equation store module is responsible for storing and loading equations along with parameters provided by the user.

All aims and objectives are successfully fulfilled for this thesis project. Set of Test Cases was created to improve the quality of the software and verify if achieved required level.

The author believes that developed application can be useful to achieve solution for ODE or system of ODE’s quickly from any device connected to the internet with web browser installed.

The developed application is currently running on Google’s App Engine and available under following address : <http://sodesolver.appspot.com/>

## Future work

The most important improvement for the future is probably adapting ODE Solvers to -th order systems and equations solving. The application was developed in such a manner, that it is easy to extend it with new features. Moreover, ODE Solver module was designed to operate on vectors instead of values with a view to -th order implementation.

Another improvement for this application could be an authentication mechanism. The idea is to create separated accounts for users operating on Equation store. Every user could store, load or remove ODE’s or systems of ODE’s which concern his account. To achieve this goal Google’s authentication mechanism could be applied, which is integrated with AppEngine.

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APPENDICES

Datastore data types



Google App Engine’s Administration console

