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Comparison of Second Order Conformal Symplectic Schemes with Linear Stability Analysis

Dwayne Floyd
University of Central Florida

COMPARISON OF SECOND ORDER CONFORMAL SYMPLECTIC SCHEMES WITH LINEAR STABILITY ANALYSIS

by

DWAYNE E. FLOYD
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ABSTRACT

Numerical methods for solving linearly damped Hamiltonian ordinary differential equations are analyzed and compared. The methods are constructed from the well-known Störmer-Verlet and implicit midpoint methods. The structure preservation properties of each method are shown analytically and numerically. Each method is shown to preserve a symplectic form up to a constant and are therefore conformal symplectic integrators, with each method shown to accurately preserve the rate of momentum dissipation. An analytical linear stability analysis is completed for each method, establishing thresholds between the value of the damping coefficient and the step-size that ensure stability. The methods are all second order and the preservation of the rate of energy dissipation is compared to that of a third order Runge-Kutta method that does not preserve conformal properties. Numerical experiments will include the damped harmonic oscillator and the damped nonlinear pendulum.

For my wife and son

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1: INTRODUCTION

For this thesis we provide a comparison between numerical methods used in modeling Hamiltonian systems with linear dissipation, generally interpreted as friction. There are many practical applications for systems of this type. As an example, it was noted in a paper by Holmberg, Andersson and Erdemir [11] that in passenger automobiles one-third of the fuel energy is used to overcome friction with 28% of the fuel energy being direct frictional losses in places such as the engine, transmission, and tires. One main objective in the design of the components of these systems would be to minimize losses due to friction and therefore increase efficiency. The dynamics of some of these mechanical systems can be well represented by a Hamiltonian with linear dissipation and it is for that purpose that the numerical methods used in the modeling of these systems and especially the modeling of the energy losses be as accurate as possible. Of particular interest would be numerical methods that will accurately preserve the rate of dissipation in the system. This practical application, as well as many others, serves as motivation for this thesis and the continual improvement in the accuracy and efficiency of the numerical methods used to model such systems.

In this thesis, we are interested in comparing numerical methods used to approximate systems of ordinary differential equations of the form, $\frac{d}{dt}z = f(z), z(t_0) = z^0 \; \epsilon \; \mathbb{R}^d$. Where $z(t_n)$ is the solution at the time t_n. We designate the approximated solution as z^n where $z^n \approx z(t_n)$ for $n \geq 0$. We typically assume the initial time $t_0 = 0$ and that all subsequent time steps are defined by $t_n = t_{n-1} + \Delta t$ for $n \geq 1$. We also assume that the solutions z^n are defined for all time steps $t \geq t_0$. In addition, we define dependent variables q and p that are used to designate column vectors of positions and momenta respectively in a Euclidean space $\mathbb{R}^d$, where d is the dimension. We utilize these notations when we apply the numerical methods to second order systems of differential equations arising from Newton's second law, $q_{tt} = f(q)$. We write the first order form of the differential equations $q_t = p$ and $p_t = g(q)$, where the time derivative of $q(t)$ is denoted by q_t and that of $p(t)$ is p_t. We next define a vector $z = [q, p]^T$ and a vector field $f(z) = \begin{bmatrix} p \\ g(q) \end{bmatrix}$. We can then apply our numerical method to the equation $z_t = f(z)$.

As shown earlier, we know there is value and practical application in being able to accurately and efficiently model the sometimes complex systems found in fields such as physics and engineering. However, with such systems it may be difficult or impractical to obtain an analytical solution because the amount of work necessary may be prohibitive to effectively model the system or establish the long term behavior of such a complex system. As noted in [1], with the exception of a few special cases, most models are not exactly integrable especially those that are nonlinear. In these situations we can apply a numerical method and obtain an approximation of the solution, or modeling of events, within an acceptable tolerance level. Of particular interest are conservative physical systems such as Hamiltonian systems, as they can be representative of a wide range of practical applications and the conservative properties of the numerical methods used to approximate such systems. Obviously, it is desirable that any numerical method used for approximating the solution offer accuracy, stability and be as efficient as possible.

The continued development of new numerical methods, improvement and modification of existing methods, and the thorough comparison of methods provides value and increases the understanding of the strengths and weaknesses of the methods available to the user. For that purpose we will provide an analysis and comparison of two types of numerical methods and apply those methods to a linear and a nonlinear ordinary differential equations. Both types of methods are structure-preserving methods and are composed from classical well know methods, those being the Störmer-Verlet method (sometimes called the leap-frog method) and the implicit midpoint method.

The construction of symplectic methods with a damping coefficient of $\gamma = 0$ can be accomplished through the process of splitting the Hamiltonian into a sum of explicitly solvable Hamiltonian vector fields [1]. A symplectic method is then created from the composition of the corresponding flow maps. Symplectic methods are structure preserving methods, that is they will exactly preserve the symplectic structure of a Hamiltonian ordinary differential equation, which is equivalent to preserving the phase space area [1]. Other invariant properties of the governing equations are also often preserved by symplectic methods, such as momentum or rotations. It has also been proven that over long time intervals symplectic methods will preserve the total energy of a system up to an exponentially small error. Due to their superior results in practice, symplectic methods are preferred by scientists and engineers for simulating conservative dynamics in many applications, such as celestial mechanics, molecular dynamics, electromagnetism, optics, and many systems that involve wave motion. A well known disadvantage to symplectic methods is they will loose orders of accuracy and structure-preserving properties when a damping coefficient of $\gamma > 0$ is introduced. For that reason, we want to extend symplectic integration to problems with damping in order to develop numerical methods that will become the preferred standard by scientists and engineers to use in applications with the presence of frictional forces.

The methods in this thesis have a damping coefficient of $\gamma > 0$ and were obtained through the construction of symplectic methods by splitting [1, 10] a process in which each of these methods has been used as the symplectic method used to approximate the conservative part of a Hamiltonian system and then composed with a exact time flow map that is used to provide the exact solution to the dissipative part of the system. A thorough description of these types of systems can be found in [6] but in simplest terms also noted in [6] they can be described as systems with coordinates (q, p), a separable Hamiltonian $H(q, p) = T(p) + V(q)$, and the following equations of motion.

$$q_t = \nabla_p T(p), \qquad p_t = -\nabla_q V(q) - 2\gamma p \tag{1.1}$$

where $q, p \ \epsilon \ \mathbb{R}^d$ and $\gamma > 0$. For these Hamiltonian systems with linear dissipation we can write them in the compact form:

$$\mathbf{J}z_t = \nabla_z H(z) - \mathbf{D}z, \tag{1.2}$$

where $z = [q,p]^T$ with $q, p \ \epsilon \ \mathbb{R}^d$, $\gamma > 0$, $\mathbf{J} = \begin{bmatrix} 0 & \textbf{-I} \\ \mathbf{I} & 0 \end{bmatrix}$, and $\mathbf{D} = 2\gamma \begin{bmatrix} 0 & \mathbf{I} \\ 0 & 0 \end{bmatrix}$ as found in [1, 8]. Through a process detailed in the work of Moore [3] the system of equations (1.1) can be written in the following form.

$$q_t = \nabla_p T(p) + \gamma q - \gamma q, \qquad p_t = -\nabla_q V(q) - \gamma p - \gamma p. \tag{1.3}$$

Utilizing these equations of motion (1.3) along with a non-separable Hamiltonian of the form

$$H_\gamma(q,p) = T(p) + V(q) + \gamma q p, \tag{1.4}$$

we note

$$\nabla_p H = \nabla_p T + \gamma q, \qquad \nabla_q H = \nabla_q V + \gamma p.$$

Therefore, utilizing this Hamiltonian (1.4) the system of equations (1.2) is equivalent to

$$\mathbf{J}z_t = \nabla_z H_\gamma(z) - \gamma \mathbf{J} z. \tag{1.5}$$

We can also show that Hamiltonian systems that can be written in the compact form (1.5) are conformal symplectic systems. We know from the work of McLachlan and Perlmutter [6] and that of Moore [3] that a differential equation $y_t = g(y)$ is said to be conformal symplectic if the following relation holds:

$$\partial_t w = -2\gamma w \quad \text{or equivalently} \quad w(t) = e^{-2\gamma t} w(0) \tag{1.6}$$

and if it is satisified for $w = dy \wedge \mathbf{J}dy$. Utilizing this definition, we show that a Hamiltonian system with linear dissipation (1.5) as shown above is conformal symplectic.

To continue we will need to utilize the following properties of the wedge product as found in [1]. Where da, db, dc are k-vectors of differential one-forms on $\Re^d$.

Skew-Symmetry: $da \wedge db = -db \wedge da$

Bilinearity: for any $\alpha, \beta \ \epsilon \ \Re^d, da \wedge (\alpha db + \beta dc) = \alpha da \wedge db + \beta da \wedge dc.$

Also, for any symmetric matrix $\mathbf{A}$, $da \wedge \mathbf{A}da = 0$.

We begin by writing the associated variational equation, where $\partial_z^2 H_\gamma$ is the Hessian matrix

$$\mathbf{J}dz_t = \partial_z^2 H_\gamma(z)dz - \gamma \mathbf{J}dz.$$

Therefore,

$$\begin{aligned} dz \wedge \mathbf{J}dz_t &= dz \wedge \partial_z^2 H_\gamma(z)dz + dz \wedge -\gamma \mathbf{J}dz, \\ dz \wedge \mathbf{J}dz_t &= dz \wedge -\gamma \mathbf{J}dz, \\ dz \wedge \mathbf{J}dz_t &= -dz \wedge \gamma \mathbf{J}dz. \end{aligned}$$

Noting that $\partial_z^2 H_\gamma(z)$ is symmetric and the wedge product is skew-symmetric.

Now taking a partial derivative,

$$\begin{aligned}\partial_t(dz \wedge \mathbf{J}dz) &= dz_t \wedge \mathbf{J}dz + dz \wedge \mathbf{J}dz_t \\ &= \mathbf{J}^T dz_t \wedge dz + dz \wedge \mathbf{J}dz_t \\ &= -dz \wedge \mathbf{J}^T dz_t + dz \wedge \mathbf{J}dz_t \\ &= dz \wedge -\mathbf{J}^T dz_t + dz \wedge \mathbf{J}dz_t \\ &= 2dz \wedge \mathbf{J}dz_t.\end{aligned}$$

Where we have utilized that the fact that
$\mathbf{J} = \begin{bmatrix} 0 & \mathbf{-I} \\ \mathbf{I} & 0 \end{bmatrix}$, $\mathbf{J}^T = \begin{bmatrix} 0 & \mathbf{I} \\ \mathbf{-I} & 0 \end{bmatrix}$ and $\mathbf{-J}^T = \begin{bmatrix} 0 & \mathbf{-I} \\ \mathbf{I} & 0 \end{bmatrix} = \mathbf{J}$

Then by Substitution,

$$\partial_t(dz \wedge \mathbf{J}dz) = -2\gamma(dz \wedge \mathbf{J}dz).$$

Again by substitution using $w = dz \wedge \mathbf{J}dz$ we have,

$$\partial_t w = -2\gamma w.$$

Therefore, we have shown that Hamiltonian systems of the form $\mathbf{J}z_t = \nabla_z H(z) - \gamma\mathbf{J}z$ satisfy the definition (1.6) of a conformal symplectic system.

We are interested in Hamiltonian systems with the presence of damping and where the symplectic form will dissipate exponentially. These systems are considered to be conformal symplectic systems [6, 3]. For this thesis we consider numerical methods that preserve such properties and are therefore considered to be conformal symplectic integrators. Numerical methods give us a way to approximate the flow-maps of a system of differential equations from one time step to another. As found in [1] any reasonable numerical method will preserve the symplecticness relation up to an error that is proportional to the local truncation error. Systems that are conservative and have a damping coefficient of $\gamma = 0$ have the symplecticness condition as found in [1]

$$dq^{n+1} \wedge dp^{n+1} = dq^n \wedge dp^n. \tag{1.7}$$

If the symplecticness condition is preserved exactly then the numerical method can be thought of as a symplectic integrator.

Systems without the presence of damping have been well studied but less is known about those systems that have a damping coefficient $\gamma > 0$. There is value in furthering the study of such systems and real-world applications that can benefit in improving the numerical methods used to approximate them, such as dissipative systems in which frictional forces are present. As defined in [3] a numerical method is a conformal symplectic integrator if the following relation holds,

$$dq^{n+1} \wedge dp^{n+1} = e^{-2\gamma\Delta t} dq^n \wedge dp^n. \tag{1.8}$$

Or, another way that this can be thought of is as found in [6] vector fields are considered conformal if their flow preserves a symplectic form up to a constant. We will show that the numerical methods in this thesis will satisify this defintion and are therefore conformal symplectic integrators.

Two of the conformal methods featured in this study have been studied and presented by others [4, 7] and both will be presented in greater detail in this thesis. In the previous work done both methods were compared analytically and numerically to well known existing numerical methods. The conformal method using the Störmer-Verlet method for the flow map of the symplectic integrator was presented as one of three integration schemes by Modin and Söderlind [7] as part of a study of the geometric integration of Hamiltonian systems perturbed by Rayleigh damping and such systems are conformal symplectic systems. It was shown that the methods in the study showed preservation of dissipation in angular momentum, and had an asymptotically correct energy dissipation rate for small values of the dissipation coefficient. In that study, the method was compared to and found to be superior to explicit Runge-Kutta methods of the same order, with numerical results using Heun's method for comparision. We will refer to this method throughout this thesis as CSV1. This method uses the formulation 1.2.

We will also use as one of numerical methods in this thesis a second conformal method developed using the Störmer-Verlet method for the flow map of the symplectic integrator. We will refer to this method as the Conformal Störmer-Verlet method-2 or CSV2. The method is referenced from the presubmission paper by Moore, Bhatt and Floyd [8] and this method uses the formulation 1.5.

The other conformal method in our study, which uses the Implicit Midpoint method for the flow map of the symplectic integrator, will be referred to throughout as the Conformal Implicit Midpoint Method [2] or CIMP. The CIMP method in this thesis is a generalization of the method that was presented in detail by Sun and Shang [4] as part of the study in structure-preserving algorithms for Birkhoffian systems. Birkhoffian systems include Hamiltonian systems with weak linear damping and therefore the results of that work are relevant to this study. The method was shown to be conformal symplectic [3] and the numerical results showed the ability to simulate the energy dissipation better than the implicit midpoint rule. Both methods have been compared to well known existing methods and found to be superior.

There are questions that arise from the studies mentioned. How does the Conformal Implicit Midpoint method compare with the Conformal Störmer-Verlet methods? Are there situations in which the explicit Störmer-Verlet methods perform as well or better than the implicit method? How do these second order methods compare to a higher order method that is not structure-preserving? Another question of interest arises from the fact that we know as the value of the damping coefficient increases the stability and or reliability of a numerical method can be in doubt. Therefore, an obvious question arises, can a relationship between the parameters of a numerical method such as step-size and the damping coefficient be derived to establish stability thresholds beyond stating ”for sufficiently small values of the damping coefficient” . A goal of this thesis is to provide answers to questions such as these. The main contributions of this thesis are:

- A comparison of the Störmer-Verlet methods with the Conformal Implicit midpoint method. Analytically we show the structure preservation properties and prove the methods are conformal symplectic integrators [3] and that the rate of momentum dissipation is preserved [1, 2, 3]. Numerically we provide a comparison of the methods when applied to a linear damped harmonic oscillator and a nonlinear damped pendulum.

- An analytical linear stability analysis will be completed for the methods by establishing the thresholds between parameters of the methods in which the eigenvalues of the method lie in the left half of the complex plane when applied to a damped harmonic oscillator, a sufficient condition for stability. The stability analysis for each method provides the correlation between the damping coefficient and the time step-size and this gives us the ability to define and understand the parameters in which the explicit conformal Störmer-Verlet methods will continue to produce acceptable results in line with those of the conformal implicit midpoint method.

- Comparison of the preservation of the rate of energy dissipation of the CIMP, CSV1 and CSV2 methods with a third order Runge-Kutta method that is not structure-preserving.

- Analytic and numerical results reveal each of the conformal methods have relatively the same level of accuracy, but the explicit methods are much more efficient.

An extension of this study would be to expand the numerical analysis to include more sophisticated ODE systems as well as PDE applications. Such an expansion would be the natural progression to give a more thorough understanding of the significance of the findings and verification that the results hold across multiple scenarios.

CHAPTER 2: NUMERICAL METHODS

The conformal symplectic methods in this thesis have been constructed by the process of Hamiltonian splitting as suggested by [1, 9, 10]. In the process of splitting the Hamiltonian part is approximated by a symplectic method $z^{i+1} = \psi_{\Delta t}(z^i)$ with $z = [q,p]^T$ and $\psi_{\Delta t}$ being the flow map of a symplectic integrator, and the non-Hamiltonian part by the exact time τ flow map [3, 1, 8]. These two flow maps are composed together to form the conformal symplectic method. We next present each of the methods and the structure preservation properties of each. We provide an example of the process involved in the construction of numerical methods with the CSV1 method.

2.1 Conformal Implicit Midpoint method

The first method presented is the Conformal Implicit Midpoint method as found in the work by Sun and Shang [4]. A generalized form of the well known Implicit midpoint method is as follows.

$$\frac{z^{n+1} - z^n}{\Delta t} = f\left(\frac{z^{n+1} + z^n}{2}\right), \tag{2.1}$$

where $z = [q,p]^T$. For the conformal form we first consider a Hamiltonian system with Hamiltonian of the form $H_\gamma(q,p) = V(q) + T(p) + \gamma qp$ with the corresponding equations of motion (1.3). Or equivalently, written in the compact form 1.5 and using the Implicit Midpoint Method (2.1) to discretize 1.5 we obtain,

$$\mathbf{J}\left(\frac{z^{n+1} - z^n}{\Delta t}\right) = \nabla H\left(\frac{z^{n+1} + z^n}{2}\right) - \gamma \mathbf{J}\left(\frac{z^{n+1} + z^n}{2}\right). \tag{2.2}$$

To form a conformal symplectic form of the implicit midpoint method we discretize the Hamiltonian part with the Implicit Midpoint Method and the non-Hamiltonian part with the exact flow map and then compose these two flow maps together we have the numerical method shown below. We will refer to this method as the CIMP method a generalized form of the method as found in the paper by Sun and Shang [4]. With $h = \Delta t$ the discretization can be written as:

$$\mathbf{J}\left(\frac{e^{\frac{\gamma h}{2}}z^{n+1} - e^{\frac{-\gamma h}{2}}z^{n}}{h}\right) = \nabla H\left(\frac{e^{\frac{\gamma h}{2}}z^{n+1} + e^{\frac{-\gamma h}{2}}z^{n}}{2}\right) \tag{2.3}$$

where $z = [q,p]^T$ with $q, p \ \epsilon \ \mathbb{R}^d$, $\gamma > 0$, $\mathbf{J} = \begin{bmatrix} 0 & \textbf{-I} \\ \mathbf{I} & 0 \end{bmatrix}$.

2.1.1 Conformal Symplecticity

In order to prove that the CIMP method is conformal symplectic it is sufficient to show that $\left(\frac{e^{\gamma h}dz^{n+1} - dz^{n}}{h}\right) \wedge \mathbf{J}\left(\frac{e^{\gamma h}dz^{n+1} + dz^{n}}{2}\right) = 0$ and then to verify that it satisfies the definition of a conformal symplectic integrator (1.8).

Theorem 2.1.1 *The Conformal Implicit Midpoint method is conformal symplectic*

Proof Writing the associated variational equation

$$\mathbf{J}\left(\frac{e^{\frac{\gamma h}{2}}dz^{n+1} - e^{\frac{-\gamma h}{2}}dz^{n}}{h}\right) = \partial_z^2 H_\gamma\left(\frac{e^{\frac{\gamma h}{2}}z^{n+1} + e^{\frac{-\gamma h}{2}}z^{n}}{2}\right)\left(\frac{e^{\frac{\gamma h}{2}}dz^{n+1} + e^{\frac{-\gamma h}{2}}dz^{n}}{2}\right)$$

Therefore,

$$\left(\frac{e^{\frac{\gamma h}{2}}dz^{n+1}+e^{\frac{-\gamma h}{2}}dz^{n}}{2}\right)\wedge\mathbf{J}\left(\frac{e^{\frac{\gamma h}{2}}dz^{n+1}-e^{\frac{-\gamma h}{2}}dz^{n}}{h}\right)=\left(\frac{e^{\frac{\gamma h}{2}}dz^{n+1}+e^{\frac{-\gamma h}{2}}dz^{n}}{2}\right)\wedge$$
$$\partial_z^2 H_\gamma\left(\frac{e^{\frac{\gamma h}{2}}z^{n+1}+e^{\frac{-\gamma h}{2}}z^{n}}{2}\right)\left(\frac{e^{\frac{\gamma h}{2}}dz^{n+1}+e^{\frac{-\gamma h}{2}}dz^{n}}{2}\right)$$
$$\left(\frac{e^{\frac{\gamma h}{2}}dz^{n+1}+e^{\frac{-\gamma h}{2}}dz^{n}}{2}\right)\wedge\mathbf{J}\left(\frac{e^{\frac{\gamma h}{2}}dz^{n+1}-e^{\frac{-\gamma h}{2}}dz^{n}}{h}\right)=0.$$

We carry out the wedge product on the left hand side to obtain,

$$\frac{e^{\frac{\gamma h}{2}}}{2}dz^{n+1}\wedge\mathbf{J}\left(\frac{e^{\frac{\gamma h}{2}}}{h}dz^{n+1}\right)+\frac{e^{\frac{\gamma h}{2}}}{2}dz^{n+1}\wedge\mathbf{J}\left(\frac{-e^{\frac{-\gamma h}{2}}}{h}dz^{n}\right)+\frac{e^{\frac{-\gamma h}{2}}}{2}dz^{n}\wedge\mathbf{J}\left(\frac{e^{\frac{\gamma h}{2}}}{h}dz^{n+1}\right)$$
$$+\frac{e^{\frac{-\gamma h}{2}}}{2}dz^{n}\wedge\mathbf{J}\left(\frac{-e^{\frac{-\gamma h}{2}}}{h}dz^{n}\right)=0$$
$$\frac{e^{\gamma h}}{2h}dz^{n+1}\wedge\mathbf{J}dz^{n+1}+\frac{-1}{2h}dz^{n+1}\wedge\mathbf{J}dz^{n}+\frac{1}{2h}dz^{n}\wedge\mathbf{J}dz^{n+1}+\frac{-e^{-\gamma h}}{2h}dz^{n}\wedge\mathbf{J}dz^{n}=0$$
$$e^{\gamma h}dz^{n+1}\wedge\mathbf{J}dz^{n+1}+-dz^{n+1}\wedge\mathbf{J}dz^{n}+dz^{n}\wedge\mathbf{J}dz^{n+1}+-e^{-\gamma h}dz^{n}\wedge\mathbf{J}dz^{n}=0$$
$$e^{\gamma h}dz^{n+1}\wedge\mathbf{J}dz^{n+1}+\text{-}\mathbf{J}^{T}dz^{n+1}\wedge dz^{n}+dz^{n}\wedge\mathbf{J}dz^{n+1}+-e^{-\gamma h}dz^{n}\wedge\mathbf{J}dz^{n}=0$$

Note, we have utilized a property of the wedge product $da\wedge(Adb)=(\mathbf{A}^{T}da)\wedge db$ for any nxn matrix **A**. Also, utilizing the fact that -$\mathbf{J}^{T}=\mathbf{J}$ we have,

$$e^{\gamma h}dz^{n+1}\wedge\mathbf{J}dz^{n+1}+\mathbf{J}dz^{n+1}\wedge dz^{n}+dz^{n}\wedge\mathbf{J}dz^{n+1}+-e^{-\gamma h}dz^{n}\wedge\mathbf{J}dz^{n}=0$$
$$e^{\gamma h}dz^{n+1}\wedge\mathbf{J}dz^{n+1}+\mathbf{J}dz^{n+1}\wedge dz^{n}+\text{-}\mathbf{J}dz^{n+1}\wedge dz^{n}+-e^{-\gamma h}dz^{n}\wedge\mathbf{J}dz^{n}=0$$
$$e^{\gamma h}dz^{n+1}\wedge\mathbf{J}dz^{n+1}+-e^{-\gamma h}dz^{n}\wedge\mathbf{J}dz^{n}=0$$
$$e^{\gamma h}dz^{n+1}\wedge\mathbf{J}dz^{n+1}=e^{-\gamma h}dz^{n}\wedge\mathbf{J}dz^{n}=0.$$

Therefore we have,

$$dz^{n+1} \wedge \mathbf{J} dz^{n+1} = e^{-2\gamma h} dz^n \wedge \mathbf{J} dz^n.$$

We have proven using the definition of conformal symplectic methods (1.8) and as defined in [3, 9, 10], that the CIMP method is conformal symplectic. ∎

To consider a specific example we provide a discretization for (1.5) with the Hamiltonian (1.4) $H_\gamma(q,p) = T(p) + V(q) + \gamma qp$. Therefore, we can write a generalized form of the method as follows:

$$\begin{aligned} q^{n+1} - e^{-\gamma h} q^n &= \frac{\gamma h}{2}\left(q^{n+1} + e^{-\gamma h} q^n\right) + \frac{h}{2}\nabla_p T\left(p^{n+1} + e^{-\gamma h} p^n\right) \\ p^{n+1} - e^{-\gamma h} p^n &= \frac{-\gamma h}{2}\left(p^{n+1} + e^{-\gamma h} p^n\right) - \frac{h}{2}\nabla_q V\left(q^{n+1} + e^{-\gamma h} q^n\right) \end{aligned} \tag{2.4}$$

Consider the ordinary differential equation for a damped harmonic oscillator

$$q_{tt} + 2\gamma q_t + \omega^2 q = 0 \tag{2.5}$$

With $T(p) = \frac{p^2}{2}$ and $V(q) = \frac{w^2 q^2}{2}$ and then with the CIMP method (2.4) being applied to (2.5), we obtain the following:

$$\begin{aligned} q^{n+1} - e^{-\gamma h} q^n &= \frac{\gamma h}{2}\left(q^{n+1} + e^{-\gamma h} q^n\right) + \frac{h}{2}\left(p^{n+1} + e^{-\gamma h} p^n\right), \\ p^{n+1} - e^{-\gamma h} p^n &= \frac{-\gamma h}{2}\left(p^{n+1} + e^{-\gamma h} p^n\right) - \frac{h\omega^2}{2}\left(q^{n+1} + e^{-\gamma h} q^n\right). \end{aligned} \tag{2.6}$$

Further, if we solve for q^{n+1} and p^{n+1} and write this method as a matrix equation we have:

$$\begin{bmatrix} q^{n+1} \\ p^{n+1} \end{bmatrix} = \left[\frac{e^{-\gamma h}}{1 - \frac{\gamma^2 h^2}{4} + \frac{h^2\omega^2}{4}}\right] \begin{bmatrix} (1+\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4} & h \\ -h\omega^2 & (1-\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4} \end{bmatrix} \begin{bmatrix} q^n \\ p^n \end{bmatrix}. \tag{2.7}$$

We can show as an example of a specific case of **Theorem 2.1.1** that this discretization does satisfy the definition of a conformal symplectic integrator (1.8).

$$dq^{n+1} \wedge dp^{n+1} = \left(\frac{e^{-\gamma h}}{1 - \frac{\gamma^2 h^2}{4} + \frac{h^2\omega^2}{4}}\right)\left[\left((1+\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4}\right)dq^n + hdp^n\right] \wedge \left(\frac{e^{-\gamma h}}{1 - \frac{\gamma^2 h^2}{4} + \frac{h^2\omega^2}{4}}\right)\left[-h\omega^2 dq^n + \left((1-\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4}\right)dp^n\right].$$

For simplicity let us define $\Phi = 1 - \frac{\gamma^2 h^2}{4} + \frac{h^2\omega^2}{4}$. Then our variational equations become

$$\begin{aligned}
dq^{n+1} \wedge dp^{n+1} &= \left(\frac{e^{-\gamma h}}{\Phi}\right)\left[\left((1+\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4}\right)dq^n + hdp^n\right] \wedge \\
&\quad \left(\frac{e^{-\gamma h}}{\Phi}\right)\left[-h\omega^2 dq^n + \left((1-\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4}\right)dp^n\right] \\
dq^{n+1} \wedge dp^{n+1} &= \left(\frac{e^{-\gamma h}}{\Phi}\right)\left((1+\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4}\right)dq^n \wedge \left(\frac{e^{-\gamma h}}{\Phi}\right)\left((1-\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4}\right)dp^n \\
&\quad + \left(\frac{e^{-\gamma h}}{\Phi}\right)(hdp^n) \wedge \left(\frac{e^{-\gamma h}}{\Phi}\right)\left(-h\omega^2 dq^n\right) \\
dq^{n+1} \wedge dp^{n+1} &= \left[\left(\frac{e^{-\gamma h}}{\Phi}\right)^2\left((1+\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4}\right)\left((1-\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4}\right)\right]dq^n \wedge dp^n \\
&\quad - \left[\left(\frac{e^{-\gamma h}}{\Phi}\right)^2 h^2\omega^2\right]dp^n \wedge dq^n \\
dq^{n+1} \wedge dp^{n+1} &= \left[\left(\frac{e^{-2\gamma h}}{\Phi^2}\right)\left((1+\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4}\right)\left((1-\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4}\right)\right]dq^n \wedge dp^n \\
&\quad + \left[\left(\frac{e^{-2\gamma h}}{\Phi^2}\right)h^2\omega^2\right]dq^n \wedge dp^n
\end{aligned}$$

continuing,

$$dq^{n+1} \wedge dp^{n+1} = \left(\frac{e^{-2\gamma h}}{\Phi^2}\right) \left[\left((1+\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4} \right) \left((1-\frac{\gamma h}{2})^2 - \frac{h^2\omega^2}{4} \right) + h^2\omega^2 \right] dq^n \wedge dp^n$$

$$dq^{n+1} \wedge dp^{n+1} = \left(\frac{e^{-2\gamma h}}{\Phi^2}\right)$$
$$\left[(1+\frac{\gamma h}{2})^2(1-\frac{\gamma h}{2})^2 + \frac{h^2\omega^2}{2}(1-\frac{\gamma h}{2})(1+\frac{\gamma h}{2}) + \frac{h^4\omega^4}{16} \right] dq^n \wedge dp^n.$$

With the previous definition of Φ it follows that

$$\Phi^2 = \left[(1+\frac{\gamma h}{2})^2(1-\frac{\gamma h}{2})^2 + \frac{h^2\omega^2}{2}(1-\frac{\gamma h}{2})(1+\frac{\gamma h}{2}) + \frac{h^4\omega^4}{16} \right].$$

Simplifying we have

$$dq^{n+1} \wedge dp^{n+1} = e^{-2\gamma h} dq^n \wedge dp^n.$$

Therefore, by the definition of conformal symplectic integrators as defined in [3] and presented in this thesis (1.8) we have shown as a specific example that the CIMP method is a conformal symplectic integrator.

2.1.2 Preservation of Angular Momentum Dissipation

We next show that the CIMP method (2.3) preserves the rate of conformal angular momentum dissipation. Consider the Hamiltonian for the N-body problem as found in [1] and with the non-separable Hamiltonian (1.4) to obtain

$$H(q,p) = \frac{1}{2}\sum_{i=1}^{N} \frac{\|p_i\|^2}{m_i} + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} \varphi_{ij}(\|q_i - q_j\|) + \gamma \sum_{i=1}^{N} q_i^T p_i. \quad (2.8)$$

This system has the corresponding equations of motion as found in [1]

$$\frac{d}{dt}q_i = \frac{1}{m_i}p_i$$
$$\frac{d}{dt}p_i = -\sum_{i\neq j}\frac{\varphi'(\|q_i - q_j\|)}{\|q_i - q_j\|}(q_i - q_j) - 2\gamma p_i.$$

We next prove that the CIMP method (2.3) preserves the rate of conformal angular momentum dissipation. We begin by noting that methods that conserve the total conformal angular momentum will satisfy the following relation.

$$\sum_{j=1}^{N}(q_j^{n+1} \times p_j^{n+1}) = e^{-2\gamma h}\sum_{j=1}^{N}(q^n \times p^n). \tag{2.9}$$

Theorem 2.1.2 *The Conformal Implicit Midpoint method (2.3) with Hamiltonian (2.8) preserves the rate of angular momentum dissipation, i.e. the method satisfies (2.9).*

Proof For simplicity let us define

$$q_j^{n+\frac{1}{2}} = \frac{1}{2}\left(e^{\frac{\gamma h}{2}}q_j^{n+1} + e^{\frac{\gamma h}{2}}q_j^n\right).$$

Writing the discrete equations for the CIMP method (2.3) we obtain

$$\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1} - e^{\frac{-\gamma h}{2}}q_j^n}{h}\Big) = \frac{1}{m_j}\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} + e^{\frac{-\gamma h}{2}}p_j^n}{2}\Big) + \gamma\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1} + e^{\frac{-\gamma h}{2}}q_j^n}{2}\Big),$$
$$\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} - e^{\frac{-\gamma h}{2}}p_j^n}{h}\Big) = -\sum_{i\neq j}\frac{\varphi_{ij}'(\|q_i^{n+\frac{1}{2}} - q_j^{n+\frac{1}{2}}\|)}{\|q_i^{n+\frac{1}{2}} - q_j^{n+\frac{1}{2}}\|}(q_j^{n+\frac{1}{2}} - q_i^{n+\frac{1}{2}}) - \gamma\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} + e^{\frac{-\gamma h}{2}}p_j^n}{2}\Big).$$

Let us define

$$\tau_{ij}^{n+\frac{1}{2}} = \frac{\varphi_{ij}^{'}(\|q_i^{n+\frac{1}{2}} - q_j^{n+\frac{1}{2}}\|)}{\|q_i^{n+\frac{1}{2}} - q_j^{n+\frac{1}{2}}\|}.$$

Then our discrete equations become

$$\begin{aligned}
\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1} - e^{\frac{-\gamma h}{2}}q_j^n}{h}\Big) &= \frac{1}{m_j}\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} + e^{\frac{-\gamma h}{2}}p_j^n}{2}\Big) + \gamma\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1} + e^{\frac{-\gamma h}{2}}q_j^n}{2}\Big),\\
\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} - e^{\frac{-\gamma h}{2}}p_j^n}{h}\Big) &= -\sum_{i\neq j}\tau_{ij}^{n+\frac{1}{2}}(q_j^{n+\frac{1}{2}} - q_i^{n+\frac{1}{2}}) - \gamma\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} + e^{\frac{-\gamma h}{2}}p_j^n}{2}\Big).
\end{aligned}$$

Now, finding the cross products and taking the sum to get the total angular momentum

$$\begin{aligned}
&\sum_{j=1}^{N}\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1} - e^{\frac{-\gamma h}{2}}q_j^n}{h}\Big) \times \Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} + e^{\frac{-\gamma h}{2}}p_j^n}{2}\Big)\\
&\quad = \sum_{j=1}^{N}\Big[\frac{1}{m_j}\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} + e^{\frac{-\gamma h}{2}}p_j^n}{2}\Big) + \gamma\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1} + e^{\frac{-\gamma h}{2}}q_j^n}{2}\Big)\Big] \times \Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} + e^{\frac{-\gamma h}{2}}p_j^n}{2}\Big)\\
&\quad = \sum_{j=1}^{N}\gamma\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1} + e^{\frac{-\gamma h}{2}}q_j^n}{2}\Big)\Big] \times \Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} + e^{\frac{-\gamma h}{2}}p_j^n}{2}\Big),
\end{aligned}$$

and then finding the next cross product

$$
\begin{aligned}
&\sum_{j=1}^{N}\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1}+e^{\frac{-\gamma h}{2}}q_j^{n}}{2}\Big)\times\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}-e^{\frac{-\gamma h}{2}}p_j^{n}}{h}\Big),\\
&=\sum_{j=1}^{N}\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1}+e^{\frac{-\gamma h}{2}}q_j^{n}}{2}\Big)\times\Big[-\sum_{i\neq j}\tau_{ij}^{n+\frac{1}{2}}(q_j^{n+\frac{1}{2}}-q_i^{n+\frac{1}{2}})-\gamma\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}+e^{\frac{-\gamma h}{2}}p_j^{n}}{2}\Big)\Big],\\
&=\sum_{j=1}^{N}q_j^{n+\frac{1}{2}}\times\Big[-\sum_{i\neq j}\tau_{ij}^{n+\frac{1}{2}}(q_j^{n+\frac{1}{2}}-q_i^{n+\frac{1}{2}})-\gamma\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}+e^{\frac{-\gamma h}{2}}p_j^{n}}{2}\Big)\Big],\\
&=\sum_{j=1}^{N}q_j^{n+\frac{1}{2}}\times\Big(-\sum_{i\neq j}\tau_{ij}^{n+\frac{1}{2}}(q_j^{n+\frac{1}{2}}-q_i^{n+\frac{1}{2}})\Big)+\sum_{j=1}^{N}q_j^{n+\frac{1}{2}}\times\gamma\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}+e^{\frac{-\gamma h}{2}}p_j^{n}}{2}\Big),\\
&=-\sum_{j=1}^{N}\sum_{i\neq j}q_j^{n+\frac{1}{2}}\times\tau_{ij}^{n+\frac{1}{2}}(q_j^{n+\frac{1}{2}}-q_i^{n+\frac{1}{2}})+\sum_{j=1}^{N}q_j^{n+\frac{1}{2}}\times\gamma\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}+e^{\frac{-\gamma h}{2}}p_j^{n}}{2}\Big),\\
&=-\sum_{j=1}^{N}\sum_{i\neq j}\tau_{ij}^{n+\frac{1}{2}}\Big(q_j^{n+\frac{1}{2}}\times q_j^{n+\frac{1}{2}}-q_j^{n+\frac{1}{2}}\times q_i^{n+\frac{1}{2}}\Big)+\sum_{j=1}^{N}q_j^{n+\frac{1}{2}}\times\gamma\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}+e^{\frac{-\gamma h}{2}}p_j^{n}}{2}\Big),\\
&=\sum_{j=1}^{N}\sum_{i\neq j}\tau_{ij}^{n+\frac{1}{2}}q_j^{n+\frac{1}{2}}\times q_i^{n+\frac{1}{2}}+\sum_{j=1}^{N}q_j^{n+\frac{1}{2}}\times\gamma\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}+e^{\frac{-\gamma h}{2}}p_j^{n}}{2}\Big).
\end{aligned}
$$

Notice, the first term can be written as a sum of pairs of terms with $i < j$

$$\tau_{ij}^{n+\frac{1}{2}}q_j^{n+\frac{1}{2}}\times q_i^{n+\frac{1}{2}}+\tau_{ji}^{n+\frac{1}{2}}q_i^{n+\frac{1}{2}}\times q_j^{n+\frac{1}{2}}$$

We also notice that $\tau_{ij}^{n+\frac{1}{2}}=\tau_{ji}^{n+\frac{1}{2}}$ as these values are only dependent upon the absolute distance between the steps. Therefore,

$$\tau_{ij}^{n+\frac{1}{2}}q_j^{n+\frac{1}{2}}\times q_i^{n+\frac{1}{2}}+\tau_{ji}^{n+\frac{1}{2}}q_i^{n+\frac{1}{2}}\times q_j^{n+\frac{1}{2}}=0,$$

and then for our cross product we have

$$\sum_{j=1}^{N}\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1}+e^{\frac{-\gamma h}{2}}q_j^n}{2}\Big)\times\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}-e^{\frac{-\gamma h}{2}}p_j^n}{h}\Big)=$$

$$-\sum_{j=1}^{N}\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1}+e^{\frac{-\gamma h}{2}}q_j^n}{2}\Big)\times\gamma\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}+e^{\frac{-\gamma h}{2}}p_j^n}{2}\Big)\Big].$$

Therefore,

$$\sum_{j=1}^{N}\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1}-e^{\frac{-\gamma h}{2}}q_j^n}{h}\Big)\times\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}+e^{\frac{-\gamma h}{2}}p_j^n}{2}\Big)+$$

$$\sum_{j=1}^{N}\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1}+e^{\frac{-\gamma h}{2}}q_j^n}{2}\Big)\times\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}-e^{\frac{-\gamma h}{2}}p_j^n}{h}\Big)=0,$$

$$\sum_{j=1}^{N}\Big[\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1}-e^{\frac{-\gamma h}{2}}q_j^n}{h}\Big)\times\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}+e^{\frac{-\gamma h}{2}}p_j^n}{2}\Big)$$

$$+\Big(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1}+e^{\frac{-\gamma h}{2}}q_j^n}{2}\Big)\times\Big(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1}-e^{\frac{-\gamma h}{2}}p_j^n}{h}\Big)\Big]=0.$$

Utilizing properties of the cross product we obtain

$$\sum_{j=1}^{N}\Big[\Big(e^{\frac{\gamma h}{2}}q_j^{n+1}-e^{\frac{-\gamma h}{2}}q_j^n\Big)\times\Big(e^{\frac{\gamma h}{2}}p_j^{n+1}+e^{\frac{-\gamma h}{2}}p_j^n\Big)+\Big(e^{\frac{\gamma h}{2}}q_j^{n+1}+e^{\frac{-\gamma h}{2}}q_j^n\Big)\times\Big(e^{\frac{\gamma h}{2}}p_j^{n+1}-e^{\frac{-\gamma h}{2}}p^n\Big)\Big]=0.$$

Expanding the cross products,

$$\sum_{j=1}^{N}\Big[e^{\gamma h}\left(q_j^{n+1}\times p_j^{n+1}\right)+\left(q_j^{n+1}\times p_j^{n}\right)-\left(q_j^{n}\times p_j^{n+1}\right)-\left(e^{-\gamma h}q_j^{n}\times p_j^{n}\right)$$
$$+\,e^{\gamma h}\left(q_j^{n+1}\times p_j^{n+1}\right)-\left(q_j^{n+1}\times p_j^{n}\right)+\left(q_j^{n}\times p_j^{n+1}\right)-e^{-\gamma h}\left(q_j^{n}\times p_j^{n}\right)\Big]=0,$$
$$\sum_{j=1}^{N}\Big[2e^{\gamma h}\left(q_j^{n+1}\times p_j^{n+1}\right)-2e^{-\gamma h}\left(q_j^{n}\times p_j^{n}\right)\Big]=0,$$
$$\sum_{j=1}^{N}2e^{\gamma h}\left(q_j^{n+1}\times p_j^{n+1}\right)=\sum_{j=1}^{N}2e^{-\gamma h}\left(q_j^{n}\times p_j^{n}\right),$$
$$\sum_{j=1}^{N}e^{\gamma h}\left(q_j^{n+1}\times p_j^{n+1}\right)=\sum_{j=1}^{N}e^{-\gamma h}\left(q_j^{n}\times p_j^{n}\right),$$
$$\sum_{j=1}^{N}\left(q_j^{n+1}\times p_j^{n+1}\right)=\sum_{j=1}^{N}e^{-2\gamma h}\left(q_j^{n}\times p_j^{n}\right).$$

Therefore, we have proven that the Conformal Implicit Midpoint method satisfies the relation for conservation of total angular momentum (2.9) because

$$\sum_{j=1}^{N}\left(q_j^{n+1}\times p_j^{n+1}\right)=e^{-2\gamma h}\sum_{j=1}^{N}\left(q_j^{n}\times p_j^{n}\right). \qquad \blacksquare$$

2.2 Conformal Störmer-Verlet methods

2.2.1 Conformal Störmer-Verlet Method-1

The next method presented is a Conformal Störmer-Verlet method as found in work by Modin and Söderlind [7]. Consider the conformal Hamiltonian system with separable Hamiltonian $H(q,p)=T(p)+V(q)$, with the corresponding equations of motion.

$$q_t=\nabla_p T(p), \qquad p_t=-\nabla_q V(q)-2\gamma p \tag{2.10}$$

where $q, p \epsilon \mathbb{R}^d$ and $\gamma > 0$. An important distinction between this Hamiltonian and the Hamiltonian used with the Conformal Implicit Midpoint method is that this Hamiltonian is separable. As found in [1, 9, 10] the equation (2.10), through the process of splitting, can be split into the Hamiltonian part and the non-Hamiltonian part. The Hamiltonian part being $q_t = \nabla_p T(p)$, $p_t = -\nabla_q V(q)$ and the non-Hamiltonian part $q_t = 0$, $p_t = -2\gamma p$. The Hamiltonian part can be approximated using the standard Störmer-Verlet method as the symplectic integrator, and the non-Hamiltonian part can be solved exactly.

The exact time flow map for the non-Hamiltonian part is

$$\Phi_\tau(q,p) = \begin{bmatrix} q \\ e^{-2\gamma\tau} p \end{bmatrix}.$$

The generalized form of the well known Störmer-Verlet method used to approximate the Hamiltonian part has the following flow map as found in [1, 7, 8] is as follows,

$$\begin{aligned} p^{n+\frac{1}{2}} &= p^n - \frac{\Delta t}{2}\nabla_q V(q^n), \\ q^{n+1} &= q^n + \Delta t \nabla_p T(p^{n+\frac{1}{2}}), \\ p^{n+1} &= p^{n+\frac{1}{2}} - \frac{\Delta t}{2}\nabla_q V(q^{n+1}). \end{aligned} \tag{2.11}$$

One way to compose the two maps is $\phi_{\Delta t} = \Phi_{\Delta t/2} \circ \Psi_{\Delta t} \circ \Phi_{\Delta t/2}$ where $\Psi_{\Delta t}$ is the time Δt flow map of the Störmer-Verlet method (2.11). Applying $\Phi_{\Delta t/2}$ to a point (q^n, p^n) of phase space, we first compute a point $(\bar{q}, \bar{p})$

$$\begin{bmatrix} \bar{q} \\ \bar{p} \end{bmatrix} = \Phi_{\Delta t/2}(q^n, p^n) = \begin{bmatrix} q^n \\ e^{-\gamma \Delta t} p^n \end{bmatrix}.$$

Apply $\Psi_{\Delta t}$ to this point to get another point $(\hat{q}, \hat{p})$

$$\begin{bmatrix} \hat{q} \\ \hat{p} \end{bmatrix} = \Psi_{\Delta t} \circ \Phi_{\Delta t/2}(q^n, p^n) = \begin{bmatrix} \bar{q} + \Delta t \nabla_p T(\bar{p} - \frac{\Delta t}{2} \nabla_q V(\bar{q})) \\ \bar{p} - \frac{\Delta t}{2} \nabla_q V(\bar{q}) - \frac{\Delta t}{2} \nabla_q V(\bar{q} + \Delta t \nabla_p T(\bar{p} - \frac{\Delta t}{2} \nabla_q V(\bar{q})) \end{bmatrix}$$

Applying $\Phi_{\Delta t/2}$ to this point gives us,

$$\begin{bmatrix} q^{n+1} \\ p^{n+1} \end{bmatrix} = \Phi_{\Delta t/2} \circ \Psi_{\Delta t} \circ \Phi_{\Delta t/2}(q^n, p^n) = \begin{bmatrix} \hat{q} \\ e^{-\gamma \Delta t} \hat{p} \end{bmatrix}.$$

Substituting for $\bar{q}$ and $\bar{p}$ gives us the numerical method as found in the work by Modin and Söderlind [7].

$$\begin{aligned} p^{n+\frac{1}{2}} &= e^{-\gamma \Delta t} p^n - \frac{\Delta t}{2} \nabla_q V(q^n), \\ q^{n+1} &= q^n + \Delta t \nabla_p T(p^{n+\frac{1}{2}}), \\ p^{n+1} &= e^{-\gamma \Delta t} \left[p^{n+\frac{1}{2}} - \frac{\Delta t}{2} \nabla_q V(q^{n+1}) \right]. \end{aligned} \tag{2.12}$$

We will reference this method as the Conformal Störmer-Verlet method-1 or CSV1.

2.2.1.1 Conformal Symplecticity

We prove that the CSV1 is a conformal symplectic method by showing that the method (2.12) satisfies the definition of a conformal symplectic integrator (1.8).

Theorem 2.2.1 *The Conformal Störmer-Verlet method (2.12) is a conformal symplectic integrator.*

Proof We begin by writing the variational equations for the method (2.12)

$$
\begin{aligned}
dp^{n+\frac{1}{2}} &= e^{-\gamma\Delta t}dp^n - \frac{\Delta t}{2}V_{qq}(q^n)dq^n,\\
dq^{n+1} &= dq^n + \Delta t dp^{n+\frac{1}{2}},\\
dp^{n+1} &= e^{-\gamma\Delta t}\Big(dp^{n+\frac{1}{2}} - \frac{\Delta t}{2}V_{qq}(q^{n+1})dq^{n+1}\Big).
\end{aligned}
$$

Again, utilizing the properties of the wedge product as noted earlier we obtain

$$
\begin{aligned}
dq^{n+1}\wedge dp^{n+1} &= dq^{n+1}\wedge e^{-\gamma\Delta t}\Big(dp^{n+\frac{1}{2}} - \frac{\Delta t}{2}V_{qq}(q^{n+1})dq^{n+1}\Big)\\
&= e^{-\gamma\Delta t}dq^{n+1}\wedge dp^{n+\frac{1}{2}}\\
&= e^{-\gamma\Delta t}\Big(dq^n + \Delta t dp^{n+\frac{1}{2}}\Big)\wedge dp^{n+\frac{1}{2}}\\
&= e^{-\gamma\Delta t}dq^n\wedge dp^{n+\frac{1}{2}}\\
&= e^{-\gamma\Delta t}dq^n\wedge\Big(e^{-\gamma\Delta t}dp^n - \frac{\Delta t}{2}V_{qq}(q^n)dq^n\Big)\\
&= e^{-\gamma\Delta t}e^{-\gamma\Delta t}dq^n\wedge dp^n\\
&= e^{-2\gamma\Delta t}dq^n\wedge dp^n.
\end{aligned}
$$

Therefore, by the definition of conformal symplectic integrators as defined in (1.8) and (1.6) we have proven that the CSV1 method is a conformal symplectic integrator. ∎

2.2.1.2 Preservation of Angular Momentum Dissipation

We next show that the method (2.12) preserves the rate of conformal angular momentum dissipation. Consider the Hamiltonian for the N-body problem as found in [1]

$$
H(q,p) = \frac{1}{2}\sum_{i=1}^{N}\frac{\|p_n\|^2}{m_i} + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\varphi_{ij}(\|q_i - q_j\|). \tag{2.13}
$$

This system has the corresponding equations of motion as found in [1]

$$\begin{aligned}\frac{d}{dt}q_i &= \frac{1}{m_i}p_i,\\ \frac{d}{dt}p_i &= -\sum_{i\neq j}\frac{\varphi^{'}(\|q_i-q_j\|)}{\|q_i-q_j\|}(q_i-q_j).\end{aligned} \tag{2.14}$$

This Hamiltonian system is in the form of $H(q,p) = T(p) + V(q)$ and therefore can be applied to the methods in this thesis that were constructed using the splitting techniques described earlier. We want to show that the method will conserve the total conformal angular momentum by proving that the relation (2.9) holds.

Theorem 2.2.2 *The Conformal Störmer-Verlet Method-1 (2.12) preserves the rate of conformal angular momentum dissipation.*

Proof Writing the discrete equations for the method (2.12) and the given Hamiltonian (2.13)

$$\begin{aligned}p_j^{n+\frac{1}{2}} &= e^{-\gamma\Delta t}p_j^n + \frac{\Delta t}{2}\sum_{i\neq j}\frac{\varphi^{'}_{ij}(\|q_i^n-q_j^n\|)}{\|q_i^n-q_j^n\|}(q_j^n-q_i^n),\\ q_j^{n+1} &= q^n + \frac{\Delta t}{m_j}(p_j^{n+\frac{1}{2}}),\\ p_j^{n+1} &= e^{-\gamma\Delta t}\left[p_j^{n+\frac{1}{2}} + \frac{\Delta t}{2}\sum_{i\neq j}\frac{\varphi^{'}_{ij}(\|q_i^{n+1}-q_j^{n+1}\|)}{\|q_i^{n+1}-q_j^{n+1}\|}(q_j^{n+1}-q_i^{n+1})\right].\end{aligned}$$

For simplicity let us define

$$\begin{aligned}\tau_{ij}^{n+1} &= \frac{\varphi^{'}_{ij}(\|q_i^{n+1}-q_j^{n+1}\|)}{\|q_i^{n+1}-q_j^{n+1}\|},\\ \tau_{ij}^{n} &= \frac{\varphi^{'}_{ij}(\|q_i^{n}-q_j^{n}\|)}{\|q_i^{n}-q_j^{n}\|}.\end{aligned} \tag{2.15}$$

Then our discrete equations become

$$
\begin{aligned}
p_j^{n+\frac{1}{2}} &= e^{-\gamma\Delta t} p_j^n + \frac{\Delta t}{2} \sum_{i \neq j} \tau_{ij}^n (q_j^n - q_i^n), \\
q_j^{n+1} &= q_j^n + \frac{\Delta t}{m_j} (p_j^{n+\frac{1}{2}}), \\
p_j^{n+1} &= e^{-\gamma\Delta t} \left[p_j^{n+\frac{1}{2}} + \frac{\Delta t}{2} \sum_{i \neq j} \tau_{ij}^{n+1} (q_j^{n+1} - q_i^{n+1}) \right].
\end{aligned}
$$

Then the total angular momentum can be found by

$$
\begin{aligned}
\sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+1} &= \sum_{j=1}^{N} q_j^{n+1} \times \left(e^{-\gamma\Delta t} \left[p_j^{n+\frac{1}{2}} + \frac{\Delta t}{2} \sum_{i \neq j} \tau_{ij}^{n+1} (q_j^{n+1} - q_i^{n+1}) \right] \right) \\
&= e^{-\gamma\Delta t} \sum_{j=1}^{N} q_j^{n+1} \times \left(\left[p_j^{n+\frac{1}{2}} + \frac{\Delta t}{2} \sum_{i \neq j} \tau_{ij}^{n+1} (q_j^{n+1} - q_i^{n+1}) \right] \right) \\
&= e^{-\gamma\Delta t} \Big[\sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+\frac{1}{2}} + \sum_{j=1}^{N} q_j^{n+1} \times \left(\frac{\Delta t}{2} \sum_{i \neq j} \tau_{ij}^{n+1} (q_j^{n+1} - q_i^{n+1}) \right) \Big] \\
&= e^{-\gamma\Delta t} \Big[\sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+\frac{1}{2}} + \frac{\Delta t}{2} \sum_{j=1}^{N} \sum_{i \neq j} q_j^{n+1} \times \tau_{ij}^{n+1} \left(q_j^{n+1} - q_i^{n+1} \right) \Big].
\end{aligned}
$$

Expanding on the second term we have,

$$
\begin{aligned}
\sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+1} &= e^{-\gamma\Delta t} \Big[\sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+\frac{1}{2}} + \frac{\Delta t}{2} \sum_{j=1}^{N} \sum_{i \neq j} \tau_{ij}^{n+1} \Big(q_j^{n+1} \times \left(q_j^{n+1} - q_i^{n+1} \right) \Big) \Big] \\
&= e^{-\gamma\Delta t} \Big[\sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+\frac{1}{2}} - \frac{\Delta t}{2} \sum_{j=1}^{N} \sum_{i \neq j} \tau_{ij}^{n+1} \Big(q_j^{n+1} \times q_i^{n+1} \Big) \Big].
\end{aligned}
$$

As shown in the proof of **Theorem 2.1.2** we have the relation,

$$
\tau_{ij}^{n+1} q_j^{n+1} \times q_i^{n+1} + \tau_{ji}^{n+1} q_i^{n+1} \times q_j^{n+1} = 0.
$$

Utilizing this result, we continue with the proof

$$\begin{aligned}
\sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+1} &= e^{-\gamma \Delta t} \sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+\frac{1}{2}} \\
&= e^{-\gamma \Delta t} \sum_{j=1}^{N} \left(q_j^n + \frac{\Delta t}{m_j} (p_j^{n+\frac{1}{2}}) \right) \times p_j^{n+\frac{1}{2}} \\
&= e^{-\gamma \Delta t} \sum_{j=1}^{N} q_j^n \times p_j^{n+\frac{1}{2}}
\end{aligned}$$

Using substitution for $p_j^{n+\frac{1}{2}}$

$$\begin{aligned}
\sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+1} &= e^{-\gamma \Delta t} \sum_{j=1}^{N} q_j^n \times \left(e^{-\gamma \Delta t} p_j^n + \frac{\Delta t}{2} \sum_{i \neq j} \tau_{ij}^n (q_j^n - q_i^n) \right), \\
&= e^{-\gamma \Delta t} \sum_{j=1}^{N} q_j^n \times e^{-\gamma \Delta t} p_j^n + e^{-\gamma \Delta t} \left(\frac{\Delta t}{2} \right) \sum_{j=1}^{N} \sum_{i \neq j} \tau_{ij}^n q_j^n \times (q_j^n - q_i^n), \\
&= e^{-2\gamma \Delta t} \sum_{j=1}^{N} q_j^n \times p_j^n - e^{-\gamma \Delta t} \left(\frac{\Delta t}{2} \right) \sum_{j=1}^{N} \sum_{i \neq j} \tau_{ij}^n q_j^n \times q_i^n.
\end{aligned}$$

We reference the proof of **Theorem 2.1.2** to show,

$$\tau_{ij}^n q_j^n \times q_i^n + \tau_{ji}^n q_i^n \times q_j^n = 0.$$

Utilizing this result, we have the desired relation and finish the proof

$$\sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+1} = e^{-2\gamma \Delta t} \sum_{j=1}^{N} q_j^n \times p_j^n.$$

Therefore, we have proven that the CSV1 method preserves the rate of dissipation of angular momentum (2.9) as defined in [1]. ∎

2.2.2 Conformal Störmer-Verlet Method-2

The next method presented in this thesis is another conformal Störmer-Verlet method. To our knowledge, this method has not been presented in a published work [8]. Similar to the Conformal Implicit Midpoint method the Hamiltonian is not separable and is of the form $H_\gamma(q,p) = V(q) + T(p) + \gamma qp$. Construction of the method requires the Hamiltonian part to be discretized with a conformal symplectic integrator and the non-Hamiltonian part with the exact flow map. The method is then constructed through a careful composition of these two flow maps. In order to distinguish this Störmer-Verlet method from (2.12) we call the method CSV2. For the discretization of the Hamiltonian part we use a generalized form of the Störmer-Verlet method or sometimes known as the generalized Leapfrog method as found in [1].

$$\begin{aligned}
p^{n+\frac{1}{2}} &= p^n - \frac{\Delta t}{2}\nabla_q H(p^{n+\frac{1}{2}}, q^n), \\
q^{n+1} &= q^n + \frac{\Delta t}{2}\left[\nabla_p H(p^{n+\frac{1}{2}}, q^n) + \nabla_p H(p^{n+\frac{1}{2}}, q^{n+1})\right], \\
p^{n+1} &= p^{n+\frac{1}{2}} - \frac{\Delta t}{2}\nabla_q H(p^{n+\frac{1}{2}}, q^{n+1}).
\end{aligned}$$

For the discretization of the non-Hamiltonian part we use the exact flow map

$$\Phi_\tau(q,p) = \begin{bmatrix} q \\ e^{-\gamma\tau} p \end{bmatrix}.$$

Using these two flow maps we construct the method that we refer to as CSV2 given by

$$\begin{aligned}\left(1+\frac{\gamma\Delta t}{2}\right)p^{n+\frac{1}{2}} &= e^{\frac{-\gamma\Delta t}{2}}p^n - \frac{\Delta t}{2}\nabla_q V(q^n),\\ \left(1-\frac{\gamma\Delta t}{2}\right)q^{n+1} &= e^{\frac{-\gamma\Delta t}{2}}\left[\left(1+\frac{\gamma\Delta t}{2}\right)e^{\frac{-\gamma\Delta t}{2}}q^n + \Delta t\nabla_p T(p^{n+\frac{1}{2}})\right],\\ p^{n+1} &= e^{\frac{-\gamma\Delta t}{2}}\left[\left(1-\frac{\gamma\Delta t}{2}\right)p^{n+\frac{1}{2}} - \frac{\Delta t}{2}\nabla_q V(q^{n+1})\right].\end{aligned} \tag{2.16}$$

2.2.2.1 Conformal Symplecticity

We now prove that the CSV2 method is conformal symplectic by showing that the method (2.16) satisfies the definition of a conformal symplectic integrator (1.8).

Theorem 2.2.3 *The CSV2 method is a conformal symplectic integrator (defined in [9]).*

Proof We begin by writing the variational equations for the method (2.12).

$$\begin{aligned}\left(1+\frac{\gamma\Delta t}{2}\right)dp^{n+\frac{1}{2}} &= e^{\frac{-\gamma\Delta t}{2}}dp^n - \frac{\Delta t}{2}V_{qq}(q^n)dq^n,\\ \left(1-\frac{\gamma\Delta t}{2}\right)dq^{n+1} &= e^{\frac{-\gamma\Delta t}{2}}\left[\left(1+\frac{\gamma\Delta t}{2}\right)e^{\frac{-\gamma\Delta t}{2}}dq^n + \Delta t T_{pp}(p^{n+\frac{1}{2}})dp^{n+\frac{1}{2}}\right],\\ dp^{n+1} &= e^{\frac{-\gamma\Delta t}{2}}\left[\left(1-\frac{\gamma\Delta t}{2}\right)dp^{n+\frac{1}{2}} - \frac{\Delta t}{2}V_{qq}(q^{n+1})dq^{n+1}\right].\end{aligned}$$

First we find, utilizing properties of the wedge product we get,

$$\begin{aligned}\left(1+\frac{\gamma\Delta t}{2}\right)dq^n\wedge dp^{n+\frac{1}{2}} &= dq^n\wedge\left[e^{\frac{-\gamma\Delta t}{2}}dp^n-\frac{\Delta t}{2}V_{qq}(q^n)dq^n\right],\\ &= dq^n\wedge e^{\frac{-\gamma\Delta t}{2}}dp^n+dq^n\wedge(-\frac{\Delta t}{2}V_{qq}(q^n)dq^n),\\ &= dq^n\wedge e^{\frac{-\gamma\Delta t}{2}}dp^n.\end{aligned}$$

Then,

$$\begin{aligned}\left(1-\frac{\gamma\Delta t}{2}\right)dp^{n+\frac{1}{2}}\wedge dq^{n+1} &= dp^{n+\frac{1}{2}}\wedge e^{\frac{-\gamma\Delta t}{2}}\left[\left(1+\frac{\gamma\Delta t}{2}\right)e^{\frac{-\gamma\Delta t}{2}}dq^n+\Delta tT_{pp}(p^{n+\frac{1}{2}})dp^{n+\frac{1}{2}}\right],\\ &= dp^{n+\frac{1}{2}}\wedge\left(e^{\frac{-\gamma\Delta t}{2}}\left(1+\frac{\gamma\Delta t}{2}\right)e^{\frac{-\gamma\Delta t}{2}}dq^n\right)\\ &+ dp^{n+\frac{1}{2}}\wedge e^{\frac{-\gamma\Delta t}{2}}\Delta tT_{pp}(p^{n+\frac{1}{2}})dp^{n+\frac{1}{2}},\\ &= e^{-\gamma\Delta t}\left(1+\frac{\gamma\Delta t}{2}\right)dp^{n+\frac{1}{2}}\wedge dq^n,\end{aligned}$$

and

$$\begin{aligned}dq^{n+1}\wedge dp^{n+1} &= dq^{n+1}\wedge e^{\frac{-\gamma\Delta t}{2}}\left(1-\frac{\gamma\Delta t}{2}\right)dp^{n+\frac{1}{2}}+dq^{n+1}\wedge -e^{\frac{-\gamma\Delta t}{2}}\frac{\Delta t}{2}V_{qq}(q^{n+1})dq^{n+1},\\ &= dq^{n+1}\wedge e^{\frac{-\gamma\Delta t}{2}}\left(1-\frac{\gamma\Delta t}{2}\right)dp^{n+\frac{1}{2}},\\ &= e^{\frac{-\gamma\Delta t}{2}}\left(1-\frac{\gamma\Delta t}{2}\right)dq^{n+1}\wedge dp^{n+\frac{1}{2}},\\ &= -e^{\frac{-\gamma\Delta t}{2}}\left(1-\frac{\gamma\Delta t}{2}\right)dp^{n+\frac{1}{2}}\wedge dq^{n+1}.\end{aligned}$$

By substitution,

$$\begin{aligned}
dq^{n+1} \wedge dp^{n+1} &= -e^{\frac{-\gamma\Delta t}{2}} \left[e^{-\gamma\Delta t} \left(1 + \frac{\gamma\Delta t}{2}\right) dp^{n+\frac{1}{2}} \wedge dq^n \right], \\
&= -e^{\frac{-3\gamma\Delta t}{2}} \left[\left(1 + \frac{\gamma\Delta t}{2}\right) dp^{n+\frac{1}{2}} \wedge dq^n \right], \\
&= e^{\frac{-3\gamma\Delta t}{2}} \left[\left(1 + \frac{\gamma\Delta t}{2}\right) dq^n \wedge dp^{n+\frac{1}{2}} \right], \\
&= e^{\frac{-3\gamma\Delta t}{2}} \left(dq^n \wedge e^{\frac{-\gamma\Delta t}{2}} dp^n \right), \\
&= e^{-2\gamma\Delta t} \left(dq^n \wedge dp^n \right).
\end{aligned}$$

We have the desired relation

$$dq^{n+1} \wedge dp^{n+1} = e^{-2\gamma\Delta t} \left(dq^n \wedge dp^n \right).$$

Therefore, by the definition of conformal symplectic integrators as defined in (1.8) we have proven that the Conformal Störmer-Verlet method-2 is a conformal symplectic integrator. ∎

2.2.2.2 Preservation of Angular Momentum Dissipation

We next show that the method (2.16) preserves the rate of conformal angular momentum dissipation. Using the same Hamiltonian for the N-Body problem (2.13) with the same corresponding equations of motion (2.14), we prove that the CSV2 method preserves the rate of conformal angular momentum dissipation by satisfying the relation (2.9).

Theorem 2.2.4 *The CSV2 method preserves the rate of conformal angular momentum dissipation.*

Proof Writing the discrete equations for the method (2.16) and the given Hamiltonian (2.13) we have

$$\left(1+\frac{\gamma\Delta t}{2}\right)p_j^{n+\frac{1}{2}} = e^{\frac{-\gamma\Delta t}{2}}p_j^n - \frac{\Delta t}{2}\sum_{i\neq j}\frac{\varphi_{ij}^{'}(\|q_i^n-q_j^n\|)}{\|q_i^n-q_j^n\|}(q_j^n-q_i^n),$$

$$\left(1-\frac{\gamma\Delta t}{2}\right)q_j^{n+1} = e^{\frac{-\gamma\Delta t}{2}}\left[\left(1+\frac{\gamma\Delta t}{2}\right)e^{\frac{-\gamma\Delta t}{2}}q_j^n + \frac{\Delta t}{m_j}(p_j^{n+\frac{1}{2}})\right],$$

$$p_j^{n+1} = e^{\frac{-\gamma\Delta t}{2}}\left[\left(1-\frac{\gamma\Delta t}{2}\right)p_j^{n+\frac{1}{2}} - \frac{\Delta t}{2}\sum_{i\neq j}\frac{\varphi_{ij}^{'}(\|q_i^{n+1}-q_j^{n+1}\|)}{\|q_i^{n+1}-q_j^{n+1}\|}(q_j^{n+1}-q_i^{n+1})\right].$$

Again, for simplicity let us use a substitution defined earlier (2.15) and substitute in τ_{ij}^{n+1} and τ_{ij}^{n+}. Therefore, our discrete equations become

$$\left(1+\frac{\gamma\Delta t}{2}\right)p_j^{n+\frac{1}{2}} = e^{\frac{-\gamma\Delta t}{2}}p_j^n - \frac{\Delta t}{2}\sum_{i\neq j}\tau_{ij}^n(q_j^n-q_i^n),$$

$$\left(1-\frac{\gamma\Delta t}{2}\right)q_j^{n+1} = e^{\frac{-\gamma\Delta t}{2}}\left[\left(1+\frac{\gamma\Delta t}{2}\right)e^{\frac{-\gamma\Delta t}{2}}q_j^n + \frac{\Delta t}{m_j}(p_j^{n+\frac{1}{2}})\right],$$

$$p_j^{n+1} = e^{\frac{-\gamma\Delta t}{2}}\left[\left(1-\frac{\gamma\Delta t}{2}\right)p_j^{n+\frac{1}{2}} - \frac{\Delta t}{2}\sum_{i\neq j}\tau_{ij}^{n+1}(q_j^{n+1}-q_i^{n+1})\right].$$

The total angular momentum can be found by

$$\begin{aligned}
\sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+1} &= \sum_{j=1}^{N} q_j^{n+1} \times \left(e^{\frac{-\gamma\Delta t}{2}} \left[\left(1 - \frac{\gamma \Delta t}{2}\right) p_j^{n+\frac{1}{2}} - \frac{\Delta t}{2} \sum_{i \neq j} \tau_{ij}^{n+1} (q_j^{n+1} - q_i^{n+1}) \right] \right), \\
&= \sum_{j=1}^{N} q_j^{n+1} \times e^{\frac{-\gamma\Delta t}{2}} \left(1 - \frac{\gamma \Delta t}{2}\right) p_j^{n+\frac{1}{2}}, \\
&= e^{\frac{-\gamma\Delta t}{2}} \left(1 - \frac{\gamma \Delta t}{2}\right) \sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+\frac{1}{2}}, \\
&= e^{\frac{-\gamma\Delta t}{2}} \left(1 - \frac{\gamma \Delta t}{2}\right) \\
&\sum_{j=1}^{N} \left(\frac{e^{\frac{-\gamma\Delta t}{2}}}{(1 - \frac{\gamma \Delta t}{2})} \left[\left(1 + \frac{\gamma \Delta t}{2}\right) e^{\frac{-\gamma\Delta t}{2}} q_j^n + \frac{\Delta t}{m_j} (p_j^{n+\frac{1}{2}}) \right] \right) \times p_j^{n+\frac{1}{2}}, \\
&= e^{\frac{-3\gamma\Delta t}{2}} \left(1 + \frac{\gamma \Delta t}{2}\right) \sum_{j=1}^{N} q_j^{n} \times p_j^{n+\frac{1}{2}}, \\
&= e^{\frac{-3\gamma\Delta t}{2}} \left(1 + \frac{\gamma \Delta t}{2}\right) \sum_{j=1}^{N} q_j^{n} \times \frac{1}{(1 + \frac{\gamma \Delta t}{2})} \left(e^{\frac{-\gamma\Delta t}{2}} p_j^n - \frac{\Delta t}{2} \sum_{i \neq j} \tau_{ij}^{n} (q_j^{n} - q_i^{n}) \right), \\
&= e^{\frac{-3\gamma\Delta t}{2}} \left(1 + \frac{\gamma \Delta t}{2}\right) \sum_{j=1}^{N} q_j^{n} \times \frac{e^{\frac{-\gamma\Delta t}{2}}}{(1 + \frac{\gamma \Delta t}{2})} p_j^n, \\
&= e^{-2\gamma\Delta t} \sum_{j=1}^{N} q_j^{n} \times p_j^n.
\end{aligned}$$

Note, we have shown earlier that in the proof of (Theorem 2.2.2) for the method CSV1 that

$$\sum_{j=1}^{N} q_j^{n+1} \times \sum_{i \neq j} \tau_{ij}^{n+1} (q_j^{n+1} - q_i^{n+1}) = 0 \text{ and } \sum_{j=1}^{N} q_j^{n} \times \sum_{i \neq j} \tau_{ij}^{n} (q_j^{n} - q_i^{n}) = 0,$$

and those steps have not been included in this proof. Therefore, we have the desired result

$$\sum_{j=1}^{N} q_j^{n+1} \times p_j^{n+1} = e^{-2\gamma\Delta t} \sum_{j=1}^{N} q_j^{n} \times p_j^n.$$

We have proven that the Conformal Störmer-Verlet method-2 preserves the rate of dissipation of angular momentum (2.9) as defined in [1]. ∎

CHAPTER 3: STABILITY ANALYSIS

As found in [1] a numerical method is asymptotically stable if the growth of the solution is asymptotically bounded. Providing a relationship between the parameters of a numerical method in which the method is asymptotically stable provides the user with the ability to understand the ranges of values available and still ensure stability. We go beyond the phrase, ”for sufficiently small values of the damping coefficient” and provide an exact relation between the step-size and the damping coefficient to ensure stability.

We can find an asymptotic stability threshold by determining the relationship between the parameters of the method in which the eigenvalues of the propagation matrix for the method are in the unit disk. We consider only linear stability, meaning we determine an asymptotic stability condition for the Conformal Störmer-Verlet methods (2.12) , (2.16) and for the Conformal Implicit Midpoint method (2.3) when applied to the damped harmonic oscillator. Comparison of the eigenvalues for the ODE with the eigenvalues for the numerical methods presented in this thesis will give a better understanding and a unique perspective on how well the methods approximate the solution.
Consider the ordinary differential equation for the damped harmonic oscillator

$$q_{tt} + 2\gamma q_t + \omega^2 q = 0. \tag{3.1}$$

If we assume initial conditions of $q(0) = 1$ and $q'(0) = 0$ and if we let $\beta = \sqrt{\omega^2 - \gamma^2}$ with $\omega > \gamma$ then we have a solution for the damped harmonic oscillator of the form.

$$q(t) = e^{-\gamma t}(cos(\beta t) + \frac{\gamma}{\beta} sin(\beta t)).$$

Now consider the conformal Hamiltonian system with separable Hamiltonian

$H(q,p) = T(p) + V(q)$, where

$$q_t = \nabla_p T(p), \qquad p_t = -\nabla_q V(q) - 2\gamma p.$$

For the damped harmonic oscillator we have $T(p) = \frac{p^2}{2}$ and $V(q) = \frac{w^2q^2}{2}$ it follows that $q_t = p$, $p_t = -w^2q - 2\gamma p$ and $q_{tt} = p_t$. We can now write the following matrix equation.

$$\begin{bmatrix} q_t \\ p_t \end{bmatrix} = e^{-\gamma t} \begin{bmatrix} 0 & 1 \\ -\omega^2 & -2\gamma \end{bmatrix} \begin{bmatrix} q \\ p \end{bmatrix},$$

with

$$q(t) = e^{-\gamma t}(cos(\beta t) + \frac{\gamma}{\beta} sin(\beta t)), \tag{3.2}$$

it follows that

$$q_t = -e^{-\gamma t}(\frac{\omega^2}{\beta})sin(\beta t).$$

We can now write the matrix equation which is a result of (3.2) and the given initial conditions

$$\begin{bmatrix} q(t) \\ p(t) \end{bmatrix} = e^{-\gamma t} \begin{bmatrix} cos(\beta t) + \frac{\gamma}{\beta} sin(\beta t) & \frac{1}{\beta} sin(\beta t) \\ \frac{-\omega^2}{\beta} sin(\beta t) & cos(\beta t) - \frac{\gamma}{\beta} sin(\beta t) \end{bmatrix} \begin{bmatrix} q_0 \\ p_0 \end{bmatrix},$$

or this matrix equation could be presented as, where **M** is called the propagation matrix for the method

$$\begin{bmatrix} q(t) \\ p(t) \end{bmatrix} = M(t) \begin{bmatrix} q_0 \\ p_0 \end{bmatrix}.$$

The eigenvalues of a $2x2$ matrix can be written in terms of the trace and the determinant as follows

$$\lambda_{\pm} = \frac{tr(M) \pm \sqrt{tr(M)^2 - 4det(M)}}{2} \tag{3.3}$$

or through simple algebraic manipulation this equation for the eigenvalues can be written as

$$\lambda_{\pm} = \frac{1}{2}tr(M) \pm \sqrt{(\frac{1}{2}tr(M))^2 - det(M)}. \tag{3.4}$$

For the simple harmonic oscillator

$$det(M) = e^{-2\gamma t}\left[(cos(\beta t) + \frac{\gamma}{\beta}sin(\beta t))(cos(\beta t) - \frac{\gamma}{\beta}sin(\beta t)) + \frac{\omega^2}{\beta^2}sin^2(\beta t)\right],$$
$$det(M) = e^{-2\gamma t}\left[cos^2(\beta t) + \frac{\omega^2 - \gamma^2}{\beta^2}sin^2(\beta t)\right].$$

With $\beta = \sqrt{\omega^2 - \gamma^2}$ then this reduces

$$det(M) = e^{-2\gamma t}. \tag{3.5}$$

It is also easily found that

$$\frac{1}{2}tr(M) = e^{-\gamma t}cos(\beta t). \tag{3.6}$$

Utilizing these relations and (3.4) we find the eigenvalues for the damped harmonic oscillator with the given initial conditions are

$$\lambda_{\pm} = e^{-\gamma t}(cos(\beta t) \pm \sqrt{cos^2(\beta t) - 1}). \tag{3.7}$$

Analysis of the eigenvalues reveals it is useful to compare values of $\frac{1}{2}tr(M)$ for each of the methods in question with the (3.7). Therefore, as an additional tool for analysis we look at the Taylor expansion of $\frac{1}{2}tr(M)$ value from (3.6) which yields

$$\frac{1}{2}tr(M) = 1 - \gamma\Delta t + \frac{1}{2}\left(2\gamma^2 - \omega^2\right)\Delta t^2 + \frac{1}{6}\left(3\gamma\omega^2 - 4\gamma^3\right)\Delta t^3$$
$$\frac{1}{24}\left(\omega^4 - 3\omega^2\gamma^2 + 3\gamma^4\right)\Delta t^4 + \frac{1}{120}\left(20\omega^2\gamma^3 - 16\gamma^5 - 5\gamma\omega^4\right)\Delta t^5 + \mathcal{O}(\Delta t^6). \quad (3.8)$$

3.1 Conformal Implicit Midpoint method

When the Conformal Implicit Midpoint method was applied to the damped harmonic oscillator (3.1), we found the matrix equation (2.7) which is stated again for simplicity.

$$\begin{bmatrix} q^{n+1} \\ p^{n+1} \end{bmatrix} = \left[\frac{e^{-\gamma\Delta t}}{1 - \frac{\gamma^2\Delta t^2}{4} + \frac{\Delta t^2\omega^2}{4}}\right] \begin{bmatrix} (1 + \frac{\gamma\Delta t}{2})^2 - \frac{\Delta t^2\omega^2}{4} & \Delta t \\ -\Delta t\omega^2 & (1 - \frac{\gamma\Delta t}{2})^2 - \frac{\Delta t^2\omega^2}{4} \end{bmatrix} \begin{bmatrix} q^n \\ p^n \end{bmatrix}$$

Utilizing the equations for the eigenvalues (3.3) and (3.4) we begin by finding the determinant

$$Det(M) = \left[\frac{e^{-2\gamma\Delta t}}{\left(1 - \frac{\gamma^2\Delta t^2}{4} + \frac{\Delta t^2\omega^2}{4}\right)^2}\right]$$
$$\left[\left((1 + \frac{\gamma\Delta t}{2})^2 - \frac{\Delta t^2\omega^2}{4}\right)\left((1 - \frac{\gamma\Delta t}{2})^2 - \frac{\Delta t^2\omega^2}{4}\right) + \Delta t^2\omega^2\right],$$
$$Det(M) = \left[\frac{e^{-2\gamma\Delta t}}{\left(1 - \frac{\gamma^2\Delta t^2}{4} + \frac{\Delta t^2\omega^2}{4}\right)^2}\right]\left(1 - \frac{\gamma^2\Delta t^2}{4} + \frac{\Delta t^2\omega^2}{4}\right)^2.$$

Therefore

$$Det(M) = e^{-2\gamma\Delta t}. \quad (3.9)$$

Next, we find $\frac{1}{2}tr(M)$

$$\frac{1}{2}tr(M) = \frac{1}{2}\left[\frac{e^{-\gamma\Delta t}}{\left(1-\frac{\gamma^2\Delta t^2}{4}+\frac{\Delta t^2\omega^2}{4}\right)}\right]\left[\left(1+\frac{\gamma\Delta t}{2}\right)^2-\frac{\Delta t^2\omega^2}{4}+\left(1-\frac{\gamma\Delta t}{2}\right)^2-\frac{\Delta t^2\omega^2}{4}\right],$$
$$\frac{1}{2}tr(M) = \frac{1}{2}\left(\frac{e^{-\gamma\Delta t}}{\left(1+\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)\right)}\right)\left(2+\frac{\gamma^2\Delta t^2}{2}-\frac{\Delta t^2\omega^2}{2}\right),$$
$$\frac{1}{2}tr(M) = \frac{1}{2}\left(\frac{e^{-\gamma\Delta t}}{\left(1+\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)\right)}\right)2\left(1+\frac{\gamma^2\Delta t^2}{4}-\frac{\Delta t^2\omega^2}{4}\right),$$
$$\frac{1}{2}tr(M) = \left(\frac{e^{-\gamma\Delta t}}{\left(1+\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)\right)}\right)\left(1-\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)\right).$$

Therefore for this method

$$\frac{1}{2}tr(M) = e^{-\gamma\Delta t}\left(\frac{1-\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}{1+\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}\right). \tag{3.10}$$

With $\lambda_\pm = \frac{1}{2}tr(M) \pm \sqrt{(\frac{1}{2}tr(M))^2 - det(M)}$ it follows that the eigenvalues for the Conformal Implicit Midpoint method are

$$\lambda_\pm = e^{-\gamma\Delta t}\left(\frac{1-\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}{1+\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}\right) \pm \sqrt{\left(e^{-\gamma\Delta t}\left(\frac{1-\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}{1+\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}\right)\right)^2 - e^{-2\gamma\Delta t}},$$
$$\lambda_\pm = e^{-\gamma\Delta t}\left(\frac{1-\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}{1+\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)} \pm \sqrt{\left(\frac{1-\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}{1+\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}\right)^2 - 1}\right),$$

or with $\beta = \sqrt{\omega^2-\gamma^2}$ and some algebraic simplification the eigenvalues can be written as

$$\lambda_\pm = e^{-\gamma\Delta t}\left(\frac{4-\Delta t^2\beta^2}{4+\Delta t^2\beta^2} \pm \sqrt{\left(\frac{4-\Delta t^2\beta^2}{4+\Delta t^2\beta^2}\right)^2 - 1}\right). \tag{3.11}$$

3.1.1 Stability Relation

A requirement for stability is $\left|\frac{1}{2}tr(M)\right| < e^{-\gamma\Delta t}$, with

$$\frac{1}{2}tr(M) = e^{-\gamma\Delta t}\left(\frac{1-\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}{1+\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}\right).$$

The stability relation requires

$$\left|e^{-\gamma\Delta t}\left(\frac{1-\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}{1+\frac{\Delta t^2}{4}\left(\omega^2-\gamma^2\right)}\right)\right| < e^{-\gamma\Delta t}.$$

Therefore we have the stability relation for the Conformal Implicit Midpoint Method

$$\frac{\Delta t^2\omega^2}{2} > \frac{\Delta t^2\gamma^2}{2} \tag{3.12}$$

The result (3.12) shows the relation can never be violated for $\omega > \gamma$ and $\Delta t > 0$ therefore, the CIMP method is unconditionally stable. This can be seen in Fig. 3.1 which shows the stability relation (3.12) holds for all values of γ if the conditions $\omega > \gamma$ and $\Delta t > 0$ are not violated.

In addition we can also look at the Taylor series expansion of $\frac{1}{2}tr(M)$ of the Conformal Implicit Midpoint method for comparison with the exact value. The Taylor series expansion of (3.10) yields

$$\begin{aligned}\frac{1}{2}tr(M) = 1 - \gamma\Delta t + \frac{1}{2}\left(2\gamma-\omega^2\right)\Delta t^2 + \frac{1}{6}\left(3\gamma\omega^2-4\gamma^3\right)\Delta t^3 \\ + \frac{1}{24}\left(10\gamma^4-12\gamma^2\omega^2+3\omega^4\right)\Delta t^4 + \frac{1}{120}\left(-26\gamma^5+40\gamma^3\omega^2-15\gamma\omega^4\right)\Delta t^5 + \mathcal{O}(\Delta t^6).\end{aligned} \tag{3.13}$$

Comparison of this Taylor series expansion (3.13) expansion with the expansion (3.8) shows

$$\frac{1}{2}tr(M) - \frac{1}{2}tr(M_{CIMP}) = \mathcal{O}(\Delta t^4).$$

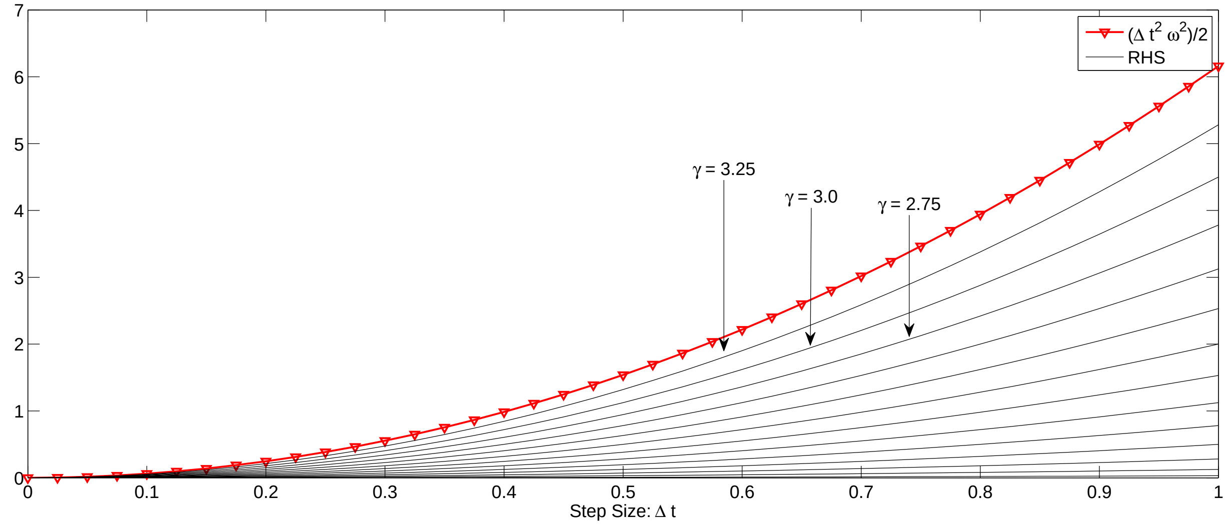

Figure 3.1: CIMP stability relation with $\gamma = 0 : .25 : 3.25$, $\Delta t = 0 : .025 : 1$ and $\omega = 3.51$

3.2 Conformal Störmer-Verlet methods

To continue the stability analysis we will also find the eigenvalues for the Conformal Störmer-Verlet methods when applied to the damped harmonic oscillator.

3.2.1 Conformal Störmer-Verlet Method-1

With $T(p) = \frac{p^2}{2}$ and $V(q) = \frac{w^2 q^2}{2}$ and then applying the CSV1 method to the ordinary differential equation for a damped harmonic oscillator (2.5) we obtain the following:

$$p^{n+\frac{1}{2}} = e^{-\gamma \Delta t} p^n - \frac{\Delta t \omega^2}{2} q^n,$$
$$q^{n+1} = q^n + \Delta t p^{n+\frac{1}{2}},$$
$$p^{n+1} = e^{-\gamma \Delta t} \left[p^{n+\frac{1}{2}} - \frac{\Delta t \omega^2}{2} q^{n+1} \right].$$

Written as a matrix equation

$$\begin{bmatrix} q^{n+1} \\ p^{n+1} \end{bmatrix} = e^{-\gamma\Delta t} \begin{bmatrix} e^{\gamma\Delta t}\left(1 - \frac{\Delta t^2\omega^2}{2}\right) & \Delta t \\ \left(\frac{\Delta t^3\omega^4}{4} - \Delta t\omega^2\right) & e^{-\gamma\Delta t}\left(1 - \frac{\Delta t^2\omega^2}{2}\right) \end{bmatrix} \begin{bmatrix} q^n \\ p^n \end{bmatrix}$$

We begin by finding the determinant

$$det(M) = e^{-2\gamma\Delta t}\left[\left(1 - \frac{\Delta t^2\omega^2}{2}\right)^2 - \left(\frac{\Delta t^4\omega^4}{4} - \Delta t^2\omega^2\right)\right],$$
$$det(M) = e^{-2\gamma\Delta t}\left[1 - \Delta t^2\omega^2 + \frac{\Delta t^4\omega^4}{4} - \frac{\Delta t^4\omega^4}{4} + \Delta t^2\omega^2\right].$$

Therefore,

$$det(M) = e^{-2\gamma\Delta t}. \tag{3.14}$$

Next, we find $\frac{1}{2}tr(M)$

$$\frac{1}{2}tr(M) = \frac{1}{2}\left(1 - \frac{\Delta t^2\omega^2}{2} + e^{-2\gamma\Delta t}\left(1 - \frac{\Delta t^2\omega^2}{2}\right)\right),$$
$$\frac{1}{2}tr(M) = \frac{1}{2}\left(1 - \frac{\Delta t^2\omega^2}{2}\right)\left(1 + e^{-2\gamma\Delta t}\right),$$
$$\frac{1}{2}tr(M) = \frac{1}{2}e^{-\gamma\Delta t}\left(1 - \frac{\Delta t^2\omega^2}{2}\right)\left(e^{\gamma\Delta t} + e^{-\gamma\Delta t}\right),$$

with $\cosh(y) = \frac{e^y + e^{-y}}{2}$ and substituting we have

$$\frac{1}{2}tr(M) = e^{-\gamma\Delta t}\left(1 - \frac{\Delta t^2\omega^2}{2}\right)\cosh(\gamma\Delta t). \tag{3.15}$$

With $\lambda_\pm = \frac{1}{2}tr(M) \pm \sqrt{(\frac{1}{2}tr(M))^2 - det(M)}$ it follows that the eigenvalues for the CSV1 method are

$$\lambda_\pm = e^{-\gamma\Delta t}\left(1 - \frac{\Delta t^2\omega^2}{2}\right)\cosh(\gamma\Delta t) \pm \sqrt{e^{-2\gamma\Delta t}\left(\left(1 - \frac{\Delta t^2\omega^2}{2}\right)^2\cosh^2(\gamma\Delta t) - 1\right)}$$
$$\lambda_\pm = e^{-\gamma\Delta t}\left[\left(1 - \frac{\Delta t^2\omega^2}{2}\right)\cosh(\gamma\Delta t) \pm \sqrt{\left(1 - \frac{\Delta t^2\omega^2}{2}\right)^2\cosh^2(\gamma\Delta t) - 1}\right]. \quad (3.16)$$

3.2.1.1 Stability Relation

Requiring $\left|\frac{1}{2}tr(M)\right| < e^{-\gamma\Delta t}$ with,

$$\frac{1}{2}tr(M) = e^{-\gamma\Delta t}\left(1 - \frac{\Delta t^2\omega^2}{2}\right)\cosh(\gamma\Delta t)$$

implies

$$\left|e^{-\gamma\Delta t}\left(1 - \frac{\Delta t^2\omega^2}{2}\right)\cosh(\gamma\Delta t)\right| < e^{-\gamma\Delta t}$$
$$-e^{-\gamma\Delta t} < e^{-\gamma\Delta t}\left(1 - \frac{\Delta t^2\omega^2}{2}\right)\cosh(\gamma\Delta t) < e^{-\gamma\Delta t}$$
$$-1 < \left(1 - \frac{\Delta t^2\omega^2}{2}\right)\cosh(\gamma\Delta t) < 1$$

Solving for $\frac{\Delta t^2\omega^2}{2}$,

$$-sech\gamma\Delta t < 1 - \frac{\Delta t^2\omega^2}{2} < sech\gamma\Delta t$$
$$-1 - sech\gamma\Delta t < -\frac{\Delta t^2\omega^2}{2} < sech\gamma\Delta t - 1$$
$$1 - sech\gamma\Delta t < \frac{\Delta t^2\omega^2}{2} < 1 + sech\gamma\Delta t$$

Therefore, we have the stability relation for the CSV1

$$1 - sech(\gamma\Delta t) < \frac{\Delta t^2\omega^2}{2} < 1 + sech(\gamma\Delta t) \tag{3.17}$$

The result (3.17) shows the relation can be violated for $\omega > \gamma$ and $\Delta t > 0$ therefore with these conditions, the CSV1 method is conditionally stable. This can be seen in Fig. 3.2 which shows the stability relation (3.17) is violated as the step-size Δt increases.

In addition we can also look at the Taylor series expansion of $\frac{1}{2}tr(M)$ of the CSV1 for comparison

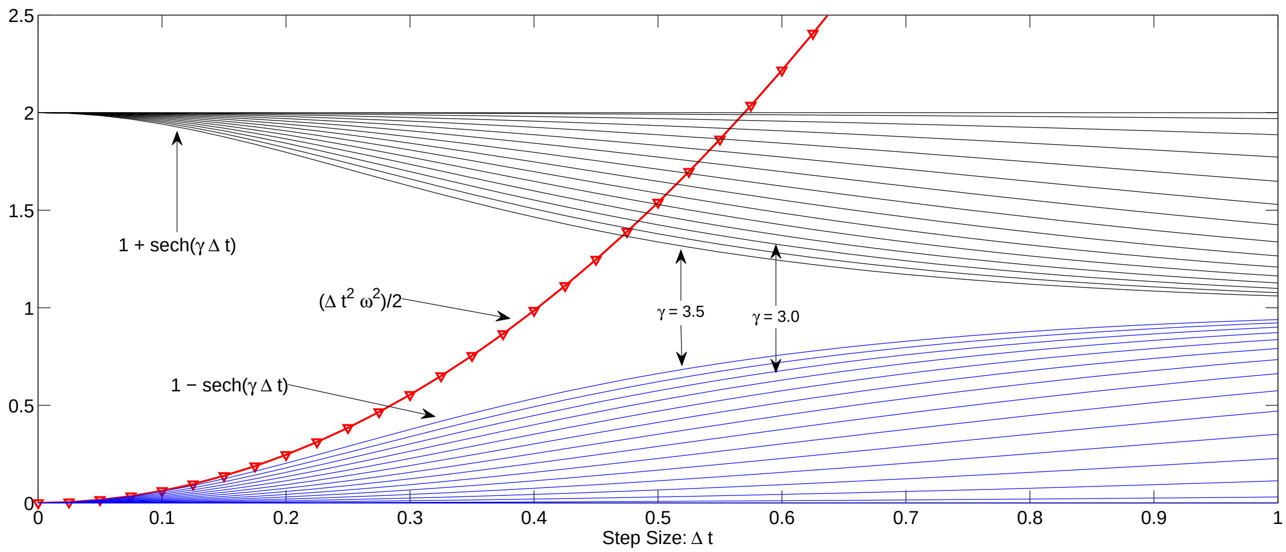

Figure 3.2: CSV1 stability relation with $\gamma = 0 : .25 : 3.5$, $\Delta t = 0 : .025 : 1$ and $\omega = 3.51$

with the exact value. Taylor expansion of (3.15) yields

$$\frac{1}{2}tr(M) = 1 - \gamma\Delta t + \frac{1}{2}\left(2\gamma^2 - \omega^2\right)\Delta t^2 + \frac{1}{6}\left(3\gamma\omega^2 - 4\gamma^3\right)\Delta t^3$$
$$+ \frac{1}{24}\left(8\gamma^4 - 12\gamma^2\omega^2\right)\Delta t^4 + \frac{1}{120}\left(40\gamma^3\omega^2 - 14\gamma^5\right)\Delta t^5 + \mathcal{O}(\Delta t^6). \tag{3.18}$$

Comparison of this Taylor series expansion (3.18) expansion with the expansion (3.8) shows

$$\frac{1}{2}tr(M) - \frac{1}{2}tr(M_{CSV1}) = \mathcal{O}(\Delta t^4).$$

3.2.2 *Conformal Störmer-Verlet Method-2*

With $T(p) = \frac{p^2}{2}$ and $V(q) = \frac{w^2q^2}{2}$ and then applying the CSV2 (2.16) to the damped harmonic oscillator (2.5) we obtain the following:

$$\begin{aligned}
\left(1+\frac{\gamma\Delta t}{2}\right)p^{n+\frac{1}{2}} &= e^{\frac{-\gamma\Delta t}{2}}p^n - \frac{\Delta t\omega^2}{2}q^n, \\
\left(1-\frac{\gamma\Delta t}{2}\right)q^{n+1} &= e^{\frac{-\gamma\Delta t}{2}}\left[\left(1+\frac{\gamma\Delta t}{2}\right)e^{\frac{-\gamma\Delta t}{2}}q^n + \Delta t(p^{n+\frac{1}{2}})\right], \\
p^{n+1} &= e^{\frac{-\gamma\Delta t}{2}}\left[\left(1-\frac{\gamma\Delta t}{2}\right)p^{n+\frac{1}{2}} - \frac{\Delta t\omega^2}{2}q^{n+1}\right].
\end{aligned}$$

Written as a matrix equation
(defining $\psi = \frac{\Delta t^3\omega^4}{2} - \Delta t\omega^2 e^{\frac{-\gamma\Delta t}{2}}\left(1+\frac{\gamma\Delta t}{2}\right)^2 - \Delta t\omega^2\left(1-\frac{\gamma\Delta t}{2}\right)^2 e^{\frac{-\gamma\Delta t}{2}}$).

$$\begin{bmatrix} q^{n+1} \\ p^{n+1} \end{bmatrix} = \frac{e^{-\gamma\Delta t}}{2\left(1-\frac{\gamma^2\Delta t^2}{4}\right)}
\begin{bmatrix} 2\left(1+\frac{\gamma\Delta t}{2}\right)^2 - \Delta t^2\omega^2 e^{\frac{-\gamma\Delta t}{2}} & 2\Delta t \\ \psi & 2\left(1-\frac{\gamma\Delta t}{2}\right)^2 - \Delta t^2\omega^2 e^{\frac{-\gamma\Delta t}{2}} \end{bmatrix}
\begin{bmatrix} q^n \\ p^n \end{bmatrix}$$

The determinant is

$$det(M) = \left(\frac{e^{-\gamma\Delta t}}{2\left(1-\frac{\gamma^2\Delta t^2}{4}\right)}\right)^2 \left[\left(2\left(1+\frac{\gamma\Delta t}{2}\right)^2 - \Delta t^2\omega^2 e^{\frac{-\gamma\Delta t}{2}}\right)\right.$$

$$\left.\left(2\left(1-\frac{\gamma\Delta t}{2}\right)^2 - \Delta t^2\omega^2 e^{\frac{-\gamma\Delta t}{2}}\right) - 2\Delta t\psi\right],$$

$$det(M) = \left(\frac{e^{-2\gamma\Delta t}}{\left(2\left(1-\frac{\gamma^2\Delta t^2}{4}\right)\right)^2}\right)\left[4\left(1+\frac{\gamma\Delta t}{2}\right)^2\left(1-\frac{\gamma\Delta t}{2}\right)^2\right].$$

Therefore,

$$det(M) = e^{-2\gamma\Delta t}. \tag{3.19}$$

Next, we find $\frac{1}{2}tr(M)$

$$\frac{1}{2}tr(M) = \frac{1}{2}\left(\frac{e^{-\gamma\Delta t}}{2\left(1-\frac{\gamma^2\Delta t^2}{4}\right)}\right)$$

$$\left(2\left(1+\frac{\gamma\Delta t}{2}\right)^2 - \Delta t^2\omega^2 e^{\frac{-\gamma\Delta t}{2}} + 2\left(1-\frac{\gamma\Delta t}{2}\right)^2 - \Delta t^2\omega^2 e^{\frac{-\gamma\Delta t}{2}}\right),$$

$$\frac{1}{2}tr(M) = \left(\frac{e^{-\gamma\Delta t}}{4\left(1-\frac{\gamma^2\Delta t^2}{4}\right)}\right)\left(4\left(1+\frac{\gamma^2\Delta t^2}{4}\right) - \Delta t^2\omega^2(e^{\frac{\gamma\Delta t}{2}} + e^{\frac{-\gamma\Delta t}{2}})\right),$$

$$\frac{1}{2}tr(M) = e^{-\gamma\Delta t}\left(\frac{\left(1+\frac{\gamma^2\Delta t^2}{4}\right)}{\left(1-\frac{\gamma^2\Delta t^2}{4}\right)} - \frac{\Delta t^2\omega^2}{2\left(1-\frac{\gamma^2\Delta t^2}{4}\right)}\cosh(\frac{\gamma\Delta t}{2})\right).$$

Therefore we have

$$\frac{1}{2}tr(M) = e^{-\gamma\Delta t}\left(\frac{4+\gamma^2\Delta t^2}{4-\gamma^2\Delta t^2} - \frac{2\Delta t^2\omega^2}{(4-\gamma^2\Delta t^2)}\cosh(\frac{\gamma\Delta t}{2})\right). \tag{3.20}$$

Defining $\phi = \left(\frac{4+\gamma^2\Delta t^2}{4-\gamma^2\Delta t^2} - \frac{2\Delta t^2\omega^2}{(4-\gamma^2\Delta t^2)}\cosh(\frac{\gamma\Delta t}{2})\right)$it follows that the eigenvalues for the CSV2 are

$$\lambda_{\pm} = e^{-\gamma\Delta t}\left(\phi \pm \sqrt{\phi^2 - 1}\right). \tag{3.21}$$

3.2.2.1 Stability Relation

Requiring $\left|\frac{1}{2}tr(M)\right| < e^{-\gamma\Delta t}$ with,

$$\frac{1}{2}tr(M) = e^{-\gamma\Delta t}\left(\frac{4+\gamma^2\Delta t^2}{4-\gamma^2\Delta t^2} - \frac{2\Delta t^2\omega^2}{(4-\gamma^2\Delta t^2)}\cosh(\frac{\gamma\Delta t}{2})\right).$$

implies

$$\begin{aligned}
&\left|e^{-\gamma\Delta t}\left(\frac{4+\gamma^2\Delta t^2}{4-\gamma^2\Delta t^2} - \frac{2\Delta t^2\omega^2}{(4-\gamma^2\Delta t^2)}\cosh(\frac{\gamma\Delta t}{2})\right)\right| < e^{-\gamma\Delta t} \\
&-e^{-\gamma\Delta t} < e^{-\gamma\Delta t}\left(\frac{4+\gamma^2\Delta t^2}{4-\gamma^2\Delta t^2} - \frac{2\Delta t^2\omega^2}{(4-\gamma^2\Delta t^2)}\cosh(\frac{\gamma\Delta t}{2})\right) < e^{-\gamma\Delta t} \\
&-1 < \left(\frac{4+\gamma^2\Delta t^2}{4-\gamma^2\Delta t^2} - \frac{2\Delta t^2\omega^2}{(4-\gamma^2\Delta t^2)}\cosh(\frac{\gamma\Delta t}{2})\right) < 1
\end{aligned}$$

Solving for $\frac{\Delta t^2\omega^2}{2}$,

$$\begin{aligned}
&\gamma^2\Delta t^2 - 4 < 4 + \gamma^2\Delta t^2 - 2\Delta t^2\omega^2 cosh(\frac{\gamma\Delta t}{2}) < 4 - \gamma^2\Delta t^2 \\
&\gamma^2\Delta t^2 - 8 < \gamma^2\Delta t^2 - 2\Delta t^2\omega^2 cosh(\frac{\gamma\Delta t}{2}) < -\gamma^2\Delta t^2 \\
&-8 < -2\Delta t^2\omega^2 cosh(\frac{\gamma\Delta t}{2}) < -2\gamma^2\Delta t^2 \\
&2\gamma^2\Delta t^2 < 2\Delta t^2\omega^2 cosh(\frac{\gamma\Delta t}{2}) < 8 \\
&\gamma^2\Delta t^2 < \Delta t^2\omega^2 cosh(\frac{\gamma\Delta t}{2}) < 4 \\
&\gamma^2\Delta t^2 sech\left(\frac{\gamma\Delta t}{2}\right) < \Delta t^2\omega^2 < 4 sech\left(\frac{\gamma\Delta t}{2}\right).
\end{aligned}$$

Therefore, we have the stability relation for the Conformal Störmer-Verlet Method-2

$$\frac{\gamma^2\Delta t^2}{2} sech\left(\frac{\gamma\Delta t}{2}\right) < \frac{\Delta t^2\omega^2}{2} < 2sech\left(\frac{\gamma\Delta t}{2}\right) \tag{3.22}$$

The result (3.22) shows the relation can be violated for $\omega > \gamma$ and $\Delta t > 0$ and therefore is conditionally stable. This can be seen in Fig. 3.3 which shows the stability relation (3.22) is violated for larger values γ as the value of the step-size Δt increases.

In addition we can also look at the Taylor series expansion of $\frac{1}{2}tr(M)$ of the Conformal Störmer-

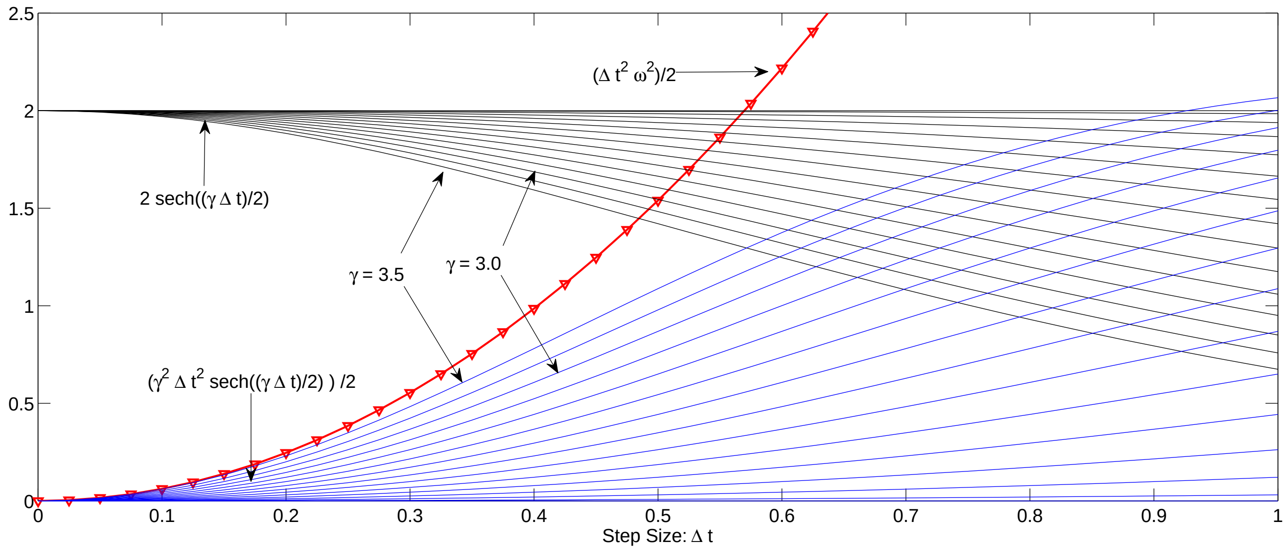

Figure 3.3: CSV2 stability relation with $\gamma = 0 : .25 : 3.5$, $\Delta t = 0 : .025 : 1$, $\omega = 3.51$

Verlet Method-2 for comparison with the exact value. Taylor expansion of (3.20) yields

$$\begin{aligned}\frac{1}{2}tr(M) &= 1 - \gamma\Delta t + \frac{1}{2}\left(2\gamma^2 - \omega^2\right)\Delta t^2 + \frac{1}{6}\left(3\gamma\omega^2 - 4\gamma^3\right)\Delta t^3 \\ &\quad + \left(\frac{5}{12}\gamma^4 - \frac{7\gamma^2\omega^2}{16}\right)\Delta t^4 + \left(\frac{13}{48}\gamma^2\omega^2 - \frac{13}{60}\gamma^4\right)\Delta t^5 + \mathcal{O}(\Delta t^6).\end{aligned} \tag{3.23}$$

Comparison of this Taylor series expansion (3.23) expansion with the expansion (3.8) shows

$$\frac{1}{2}tr(M) - \frac{1}{2}tr(M_{CSV2}) = \mathcal{O}(\Delta t^4).$$

In the stability analysis we found the exact eigenvalues for the damped harmonic oscillator (3.7). Applying each of the numerical methods to the damped harmonic oscillator example we also found the eigenvalues for the CSV1 method (3.16), the eigenvalues for the CSV2 method (3.21) and for the CIMP method (3.11). Analysis of the eigenvalue equation (3.4) shows that the accuracy of the approximated eigenvalues from each of the methods is dependent upon how well each of the methods approximate the value of $\frac{1}{2}tr(M)$ as the determinant for each of the methods was found to be the same. The error in $\frac{1}{2}tr(M)$ for each of the methods is seen in Fig. 3.4 for various values of γ. The $\frac{1}{2}tr(M)$ error seen in Fig. 3.4 is calculated as

$$\frac{1}{2}tr(M)Error = |\frac{1}{2}tr(M) - \frac{1}{2}tr(M_{num})|.$$

For small values of γ we see in Fig. 3.4 that the CSV1 method and the CSV2 method perform only slightly better at approximating $\frac{1}{2}tr(M)$ than the CIMP method. As gamma grows large enough we see a crossing of the values such that the Conformal Implicit Midpoint method performs better at the approximation of $\frac{1}{2}tr(M)$.

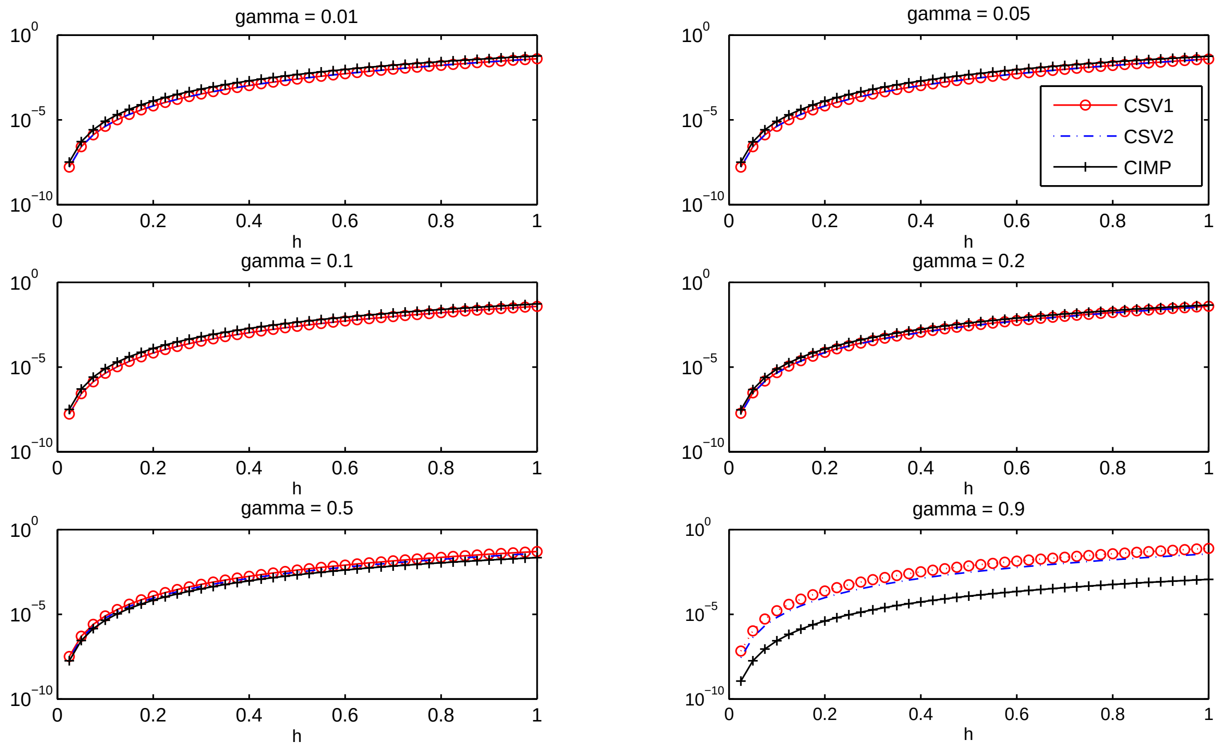

Figure 3.4: $\frac{1}{2}tr(M)$ error of approximated eigenvalues with $h = 0$ to 1 with $\Delta t = .025, \omega = 1$.

CHAPTER 4: NUMERICAL EXPERIMENTS

4.1 Damped Harmonic Oscillator

For a numerical example let us again consider the damped harmonic oscillator (2.5), given by

$$q_{tt} + 2\gamma q_t + \omega^2 q = 0.$$

With $T(p) = \frac{p^2}{2}$ and $V(q) = \frac{w^2 q^2}{2}$, we apply each of the numerical methods in this thesis to the equation.

Applying the CSV1 method to the damped harmonic oscillator (2.5) we obtain the following system:

$$\begin{aligned} p^{n+\frac{1}{2}} &= e^{-\gamma\Delta t} p^n - \frac{\Delta t \omega^2}{2} q^n, \\ q^{n+1} &= q^n + \Delta t p^{n+\frac{1}{2}}, \\ p^{n+1} &= e^{-\gamma\Delta t} \left[p^{n+\frac{1}{2}} - \frac{\Delta t \omega^2}{2} q^{n+1} \right]. \end{aligned} \tag{4.1}$$

Also, applying the CSV2 method to the damped harmonic oscillator (2.5), we obtain the following system:

$$\begin{aligned} \left(1 + \frac{\gamma\Delta t}{2}\right) p^{n+\frac{1}{2}} &= e^{\frac{-\gamma\Delta t}{2}} p^n - \frac{\Delta t \omega^2}{2} q^n, \\ \left(1 - \frac{\gamma\Delta t}{2}\right) q^{n+1} &= e^{\frac{-\gamma\Delta t}{2}} \left[\left(1 + \frac{\gamma\Delta t}{2}\right) e^{\frac{-\gamma\Delta t}{2}} q^n + \Delta t (p^{n+\frac{1}{2}}) \right], \\ p^{n+1} &= e^{\frac{-\gamma\Delta t}{2}} \left[\left(1 - \frac{\gamma\Delta t}{2}\right) p^{n+\frac{1}{2}} - \frac{\Delta t \omega^2}{2} q^{n+1} \right]. \end{aligned} \tag{4.2}$$

And, applying the CIMP method to the damped harmonic oscillator (2.5), we obtain the following:

$$q^{n+1} - e^{-\gamma\Delta t} q^n = \frac{\gamma\Delta t}{2}\left(q^{n+1} + e^{-\gamma\Delta t} q^n\right) + \frac{\Delta t}{2}\left(p^{n+1} + e^{-\gamma\Delta t} p^n\right),$$
$$p^{n+1} - e^{-\gamma\Delta t} p^n = \frac{-\gamma\Delta t}{2}\left(p^{n+1} + e^{-\gamma\Delta t} p^n\right) - \frac{\Delta t\omega^2}{2}\left(q^{n+1} + e^{-\gamma\Delta t} q^n\right). \tag{4.3}$$

Utilizing these systems of equations (4.1,4.2,4.3) as the algorithms for the approximation of the

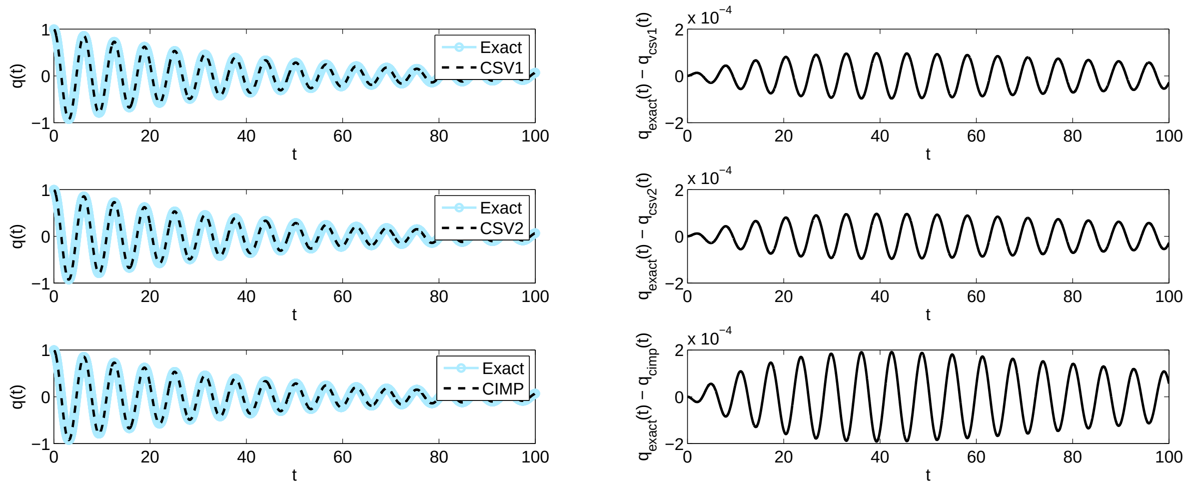

Figure 4.1: Numerical solutions $q(t)$ vs. Exact for $\Delta t = .0125, \gamma = .025$ and $\omega = 1$.

solution of the damped harmonic oscillator (2.5) we obtain the results as seen in Fig. 4.1. From Fig. 4.1, in each row the graph on the left represents the numerical solution $q(t)$ plotted with the exact solution and the graph of the right represents the difference $q_{exact}(t) - q_{approx}(t)$ for each of the methods in this thesis. The top row represents the numerical solution of the CSV1 method plotted with the exact solution, the second row represents the numerical solution of the CSV2 method and the third row represents the CIMP method. Using the graphs on the left in Fig. 4.1, we can see that each of these algorithms approximates the solution of the damped harmonic oscillator well and on the right we see that the plots of the difference $q_{exact}(t) - q_{approx}(t)$ show the CSV1 and CSV2 methods with nearly equal results and approximating the solution $q(t)$ slightly better than the CIMP method.

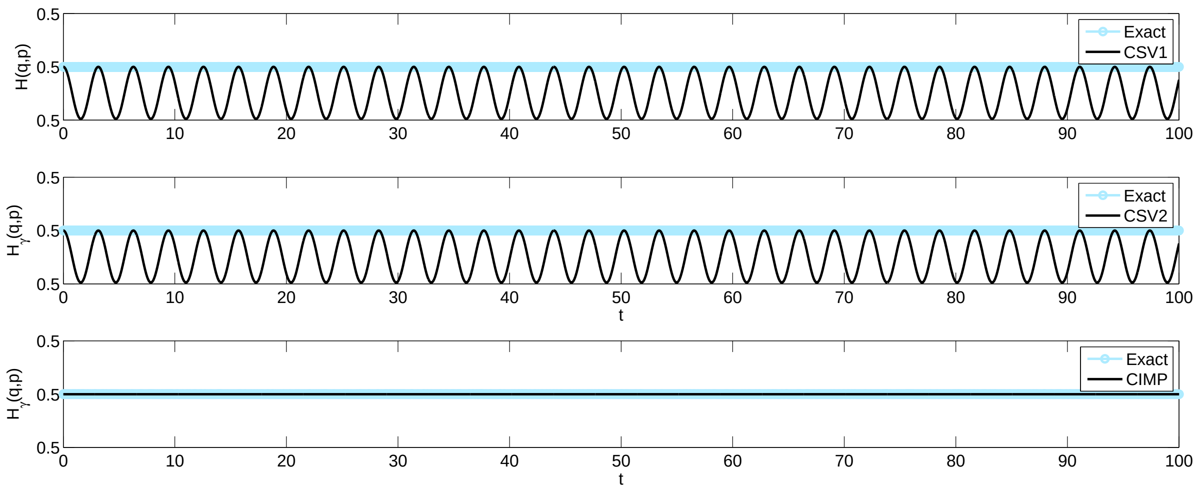

Figure 4.2: Energy H(q,p) comparisons with $\Delta t = .0125, \gamma = 0.0$ and $\omega = 1$.

To provide further verification of the analytical results and to verify conservative properties of the CSV1, CSV2 and CIMP methods we check the total energy when applied to the damped harmonic oscillator (3.1) with $\gamma = 0$. We see in Fig. 4.2 that the total energy for the CSV1 and CSV2 methods stays within a band for $\gamma = 0$, while the CIMP method the total energy is exact. For the 2^{nd} order CIMP method total energy is exactly preserved because the problem is linear and for the CSV1 and CSV2 methods, the total energy is nearly conserved with $\gamma = 0$. In Fig. 4.3 for $\gamma > 0$, the graphs on the left show a comparison of the exact total energy with that of the numerical method, and on the right we show the difference $H_{exact}(q,p) - H_{approx}(q,p)$. As with the approximation of the solution in Fig. 4.1, it appears that each of the methods (4.1,4.2,4.3) also do well in the approximation of the total energy of the system as seen on the graphs on the left in Fig. 4.3. The graphs on the right in Fig. 4.3 show the difference $H_{exact}(q,p) - H_{approx}(q,p)$ for the CSV1 (4.1) and CSV2 (4.2) methods to be essentially equal. The difference $H_{exact}(q,p) - H_{approx}(q,p)$ for

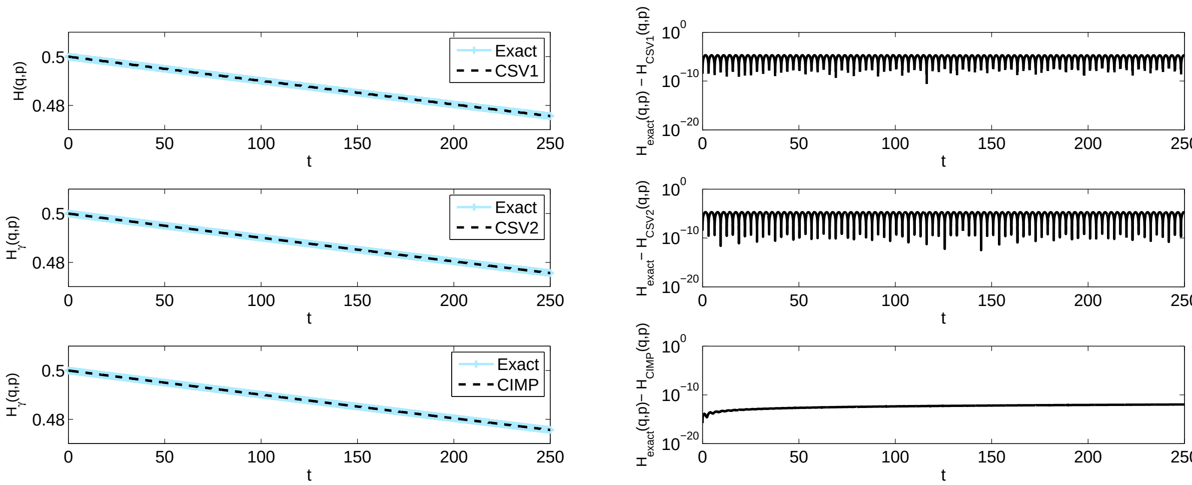

Figure 4.3: Energy H(q,p) comparisons with $\Delta t = .0125, \gamma = .0001$ and $\omega = 1$.

the CIMP (4.3) method is seen to be essentially zero.

To examine further how well these numerical schemes (4.1,4.2,4.3) approximate the solution of the damped harmonic oscillator and to provide a more accurate comparison between them, we will examine the error in the numerical approximations of the exact solution. To accomplish the comparison of the error in the approximations we look at the relative error between the approximation and the exact solution for various values of γ as seen in Fig. 4.4. In Fig. 4.4 we see that in the long time that the CIMP, CSV1 and CSV2 methods have basically the same relative error. The relative error is calculated as $|U - u| / |u|$ where U is the approximated solution and u is the exact solution. In Fig. 4.4 we see that for small values of γ the CSV1 method and the CSV2 method have slightly lower relative error than the CIMP method, as seen in the top row and second row left of Fig. 4.4. As γ increases we see a narrowing of the differences between the methods until the initial relative error is better with the CIMP method than with the other two methods. This pattern continues as γ increases with the time required for this crossing of the relative error values to occur increasing as well until eventually γ has reached a high enough value to where the crossing of the graphs does not occur and the relative error in the CIMP method is better than the relative error in the other two methods and this is seen in Fig. 4.4 bottom right.

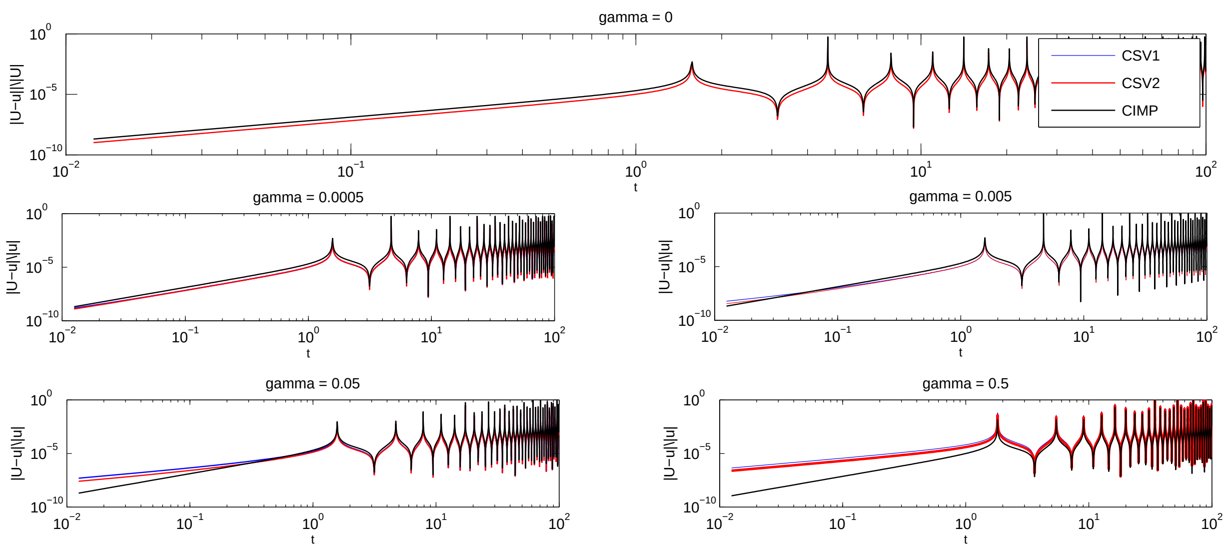

Figure 4.4: Relative Error $|U-u|\ /|u|$ with $\Delta t = .0125, \omega = 1$.

We have shown in the Fig. 4.2 the total energy $H(q,p)$ with $\gamma = 0$. In Fig. 4.5 we add a comparison with a higher order method, the 3rd order Runge-Kutta method (RK3). As in Fig. 4.2, for the 2^{nd} order CIMP method total energy is exactly preserved because the problem is linear and for the CSV1 and CSV2 methods, the total energy is nearly conserved with $\gamma = 0$, as seen in the top graph of Fig. 4.5. The 3rd order Runge-Kutta shows it does not possess the conservative properties of the CSV1, CSV2 and CIMP methods, and can not produce good results despite being a higher order method. Further verification can be seen in the bottom graph of Fig. 4.5, where we look at the difference $H_{exact}(q,p) - H_{approx}(q,p)$. The bottom graph in Fig. 4.5 shows a clear drift in the total energy $H(q,p)$ for the 3rd order Runge-Kutta method when $\gamma > 0$ that is not seen with the other methods (4.1,4.2,4.3).

For the preservation of the rate of energy dissipation we initially look at a comparison of the phase

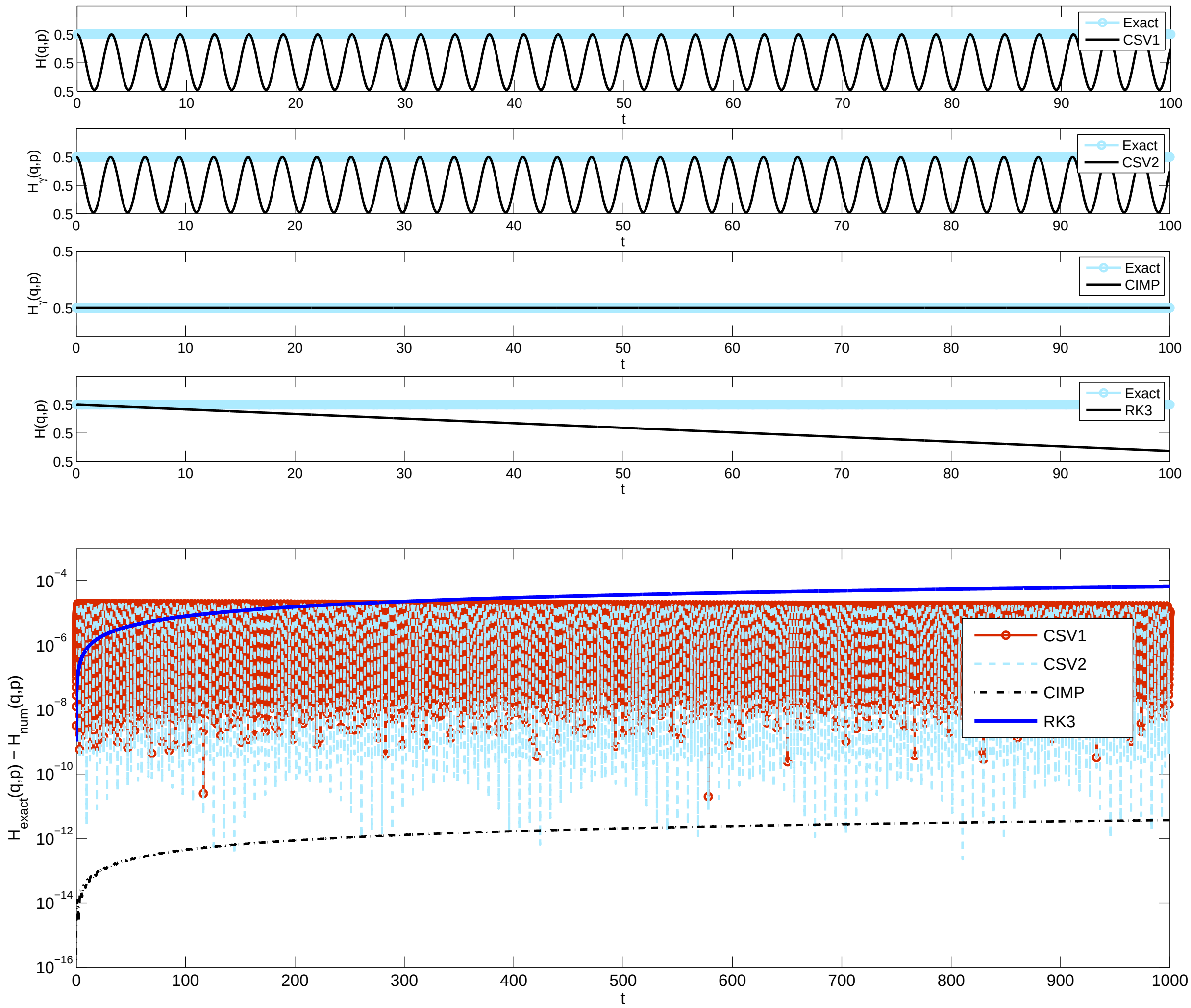

Figure 4.5: Energy H(q,p) with $\Delta t = .0125, \omega = 1$ top: $\gamma = 0$ bottom:$\gamma = .0001$

diagrams for each of the methods. It was noted that the CSV1, CSV2, and the CIMP methods all appear to not be impacted to a great extent by the step size chosen. However, as seen in Fig. 4.6 the rate of dissipation in the 3rd order Runge-Kutta method was shown to be dependent upon the step size. As the step size increased we see a significant difference in the size of the hole in the middle of the phase diagrams of the 3rd order Runge-Kutta method as compared to the CSV1,CSV2 and Conformal Implicit Midpoint method, indicating a difference in the rate of dissipation. For further

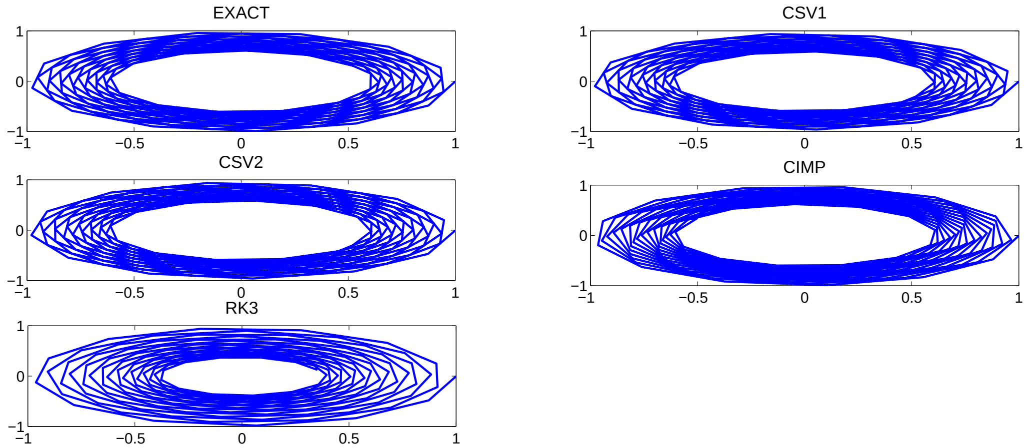

Figure 4.6: Phase space graphs $q(t)$ vs $p(t)$ with $\Delta t = .5$ and $\gamma = .005$.

verification of the results in the rate of energy dissipation as seen in Fig. 4.6 we consider the function

$$d(t) = ln\,(max(U(t))) + \gamma t, \tag{4.4}$$

where $U(t)$ denotes the numerical solution. In Fig. 4.7 we see the plots of $d(t)$ for the CSV1, CSV2, CIMP and the 3rd order Runge-Kutta methods. It is noted in Fig. 4.7 that no drift is present in the CSV1, CSV2 and the CIMP methods, while there is a clear drift in the dissipation rate for the 3rd order Runge-Kutta method. This is an important result as the CSV1, CSV2, and CIMP methods are second order methods and show preservation of the rate of dissipation of the energy while the 3rd order Runge-Kutta method shows a clear drift in the rate of dissipation.

We conclude from the these results that methods with higher order truncation error are not necessarily more accurate, and numerical structure-preservation is an important consideration even for dissipative systems.

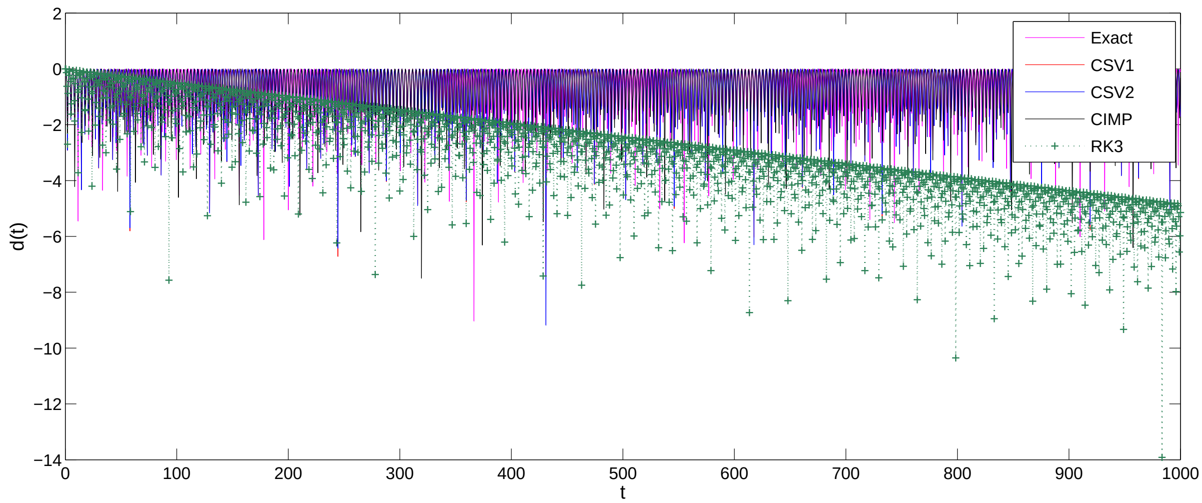

Figure 4.7: Drift in rate of energy dissipation $d(t)$with $\Delta t = .5$ and $\gamma = .005$.

4.2 Damped Nonlinear Pendulum

As a second numerical example let us consider the ordinary differential equation for a damped nonlinear pendulum, given by

$$q_{tt} + 2\gamma q + sin(q) = 0. \tag{4.5}$$

With $T(p) = \frac{p^2}{2}$ and $V(q) = -\cos q$ we apply the CSV1,CSV2, and the CIMP methods to the equation of the damped nonlinear pendulum. For the CSV1 method when applied to the damped nonlinear pendulum (4.5) we have the following system of equations:

$$\begin{aligned} p^{n+\frac{1}{2}} &= e^{-\gamma\Delta t}p^n - \frac{\Delta t}{2}\sin q^n, \\ q^{n+1} &= q^n + \Delta t p^{n+\frac{1}{2}}, \\ p^{n+1} &= e^{-\gamma\Delta t}\left[p^{n+\frac{1}{2}} - \frac{\Delta t}{2}\sin q^{n+1}\right]. \end{aligned} \tag{4.6}$$

Applying the CSV2 method to (4.5) we obtain the following system of equations:

$$\begin{aligned}\left(1+\frac{\gamma\Delta t}{2}\right)p^{n+\frac{1}{2}} &= e^{\frac{-\gamma\Delta t}{2}}p^n - \frac{\Delta t}{2}\sin\left(q^n\right),\\ \left(1-\frac{\gamma\Delta t}{2}\right)q^{n+1} &= e^{\frac{-\gamma\Delta t}{2}}\left[\left(1+\frac{\gamma\Delta t}{2}\right)e^{\frac{-\gamma\Delta t}{2}}q^n + \Delta t(p^{n+\frac{1}{2}})\right],\\ p^{n+1} &= e^{\frac{-\gamma\Delta t}{2}}\left[\left(1-\frac{\gamma\Delta t}{2}\right)p^{n+\frac{1}{2}} - \frac{\Delta t}{2}\sin\left(q^{n+1}\right)\right].\end{aligned} \tag{4.7}$$

And when we apply the CIMP method to (4.5) we have the following system of equations:

$$\begin{aligned}\left(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1} - e^{\frac{-\gamma h}{2}}q_j^n}{h}\right) &= \left(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} + e^{\frac{-\gamma h}{2}}p_j^n}{2}\right) + \gamma\left(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1} + e^{\frac{-\gamma h}{2}}q_j^n}{2}\right),\\ \left(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} - e^{\frac{-\gamma h}{2}}p_j^n}{h}\right) &= -\sin\left(\frac{e^{\frac{\gamma h}{2}}q_j^{n+1} + e^{\frac{-\gamma h}{2}}q_j^n}{2}\right) - \gamma\left(\frac{e^{\frac{\gamma h}{2}}p_j^{n+1} + e^{\frac{-\gamma h}{2}}p_j^n}{2}\right).\end{aligned} \tag{4.8}$$

Due to the complexity of using the actual exact solution for comparison with our approximated solutions from the methods in question, we used for the exact solution a 4th order Runge-Kutta-Fehlberg method approximation of the solution with thresholds set to ensure that the solution error was bounded between $1.0e^{-10}$ and $1.0e^{-12}$. We will refer to this numerical solution as the ”exact” solution.

Utilizing these systems of equations (4.6,4.7,4.8) as algorithms for the approximation of the solution of the damped nonlinear pendulum (4.5) we obtain the results seen in Fig. 4.8. In Fig. 4.8, on the left we see the exact solution plotted with the numerical solution $q(t)$ for each of the methods and on the right we see the difference $q_{exact}(t) - q_{approx}(t)$. The results in Fig. 4.8 show the difference $q_{exact}(t) - q_{approx}(t)$ for each numerical method to be equal.

For another observation on the effectiveness of the CSV1, CSV2 and CIMP methods in approximating the solution we consider the phase space graph of the nonlinear pendulum with the presence of damping as seen in Fig. 4.9. In this figure, we use a time step size of $\Delta t = .025$ and for the

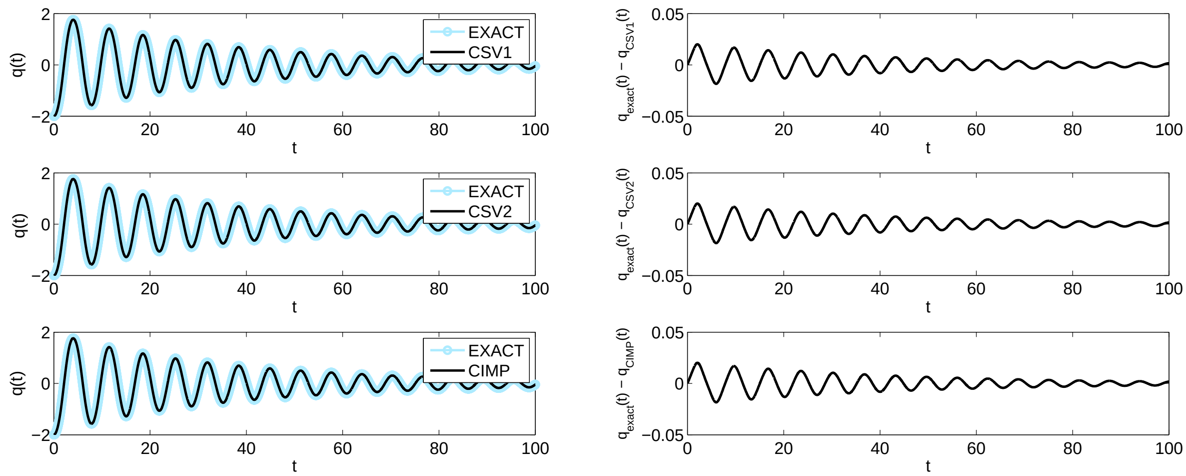

Figure 4.8: Pendulum: Numerical Solutions $q(t)$ vs Exact for $\Delta t = .0125, \gamma = .025$

damping coefficient a value of $\gamma = .05$. We see in Fig. 4.9 that with the given initial conditions and the parameters noted earlier, an exponential decay of the motion of the pendulum towards the origin, an effect of the damping of this pendulum. It appears in Fig. 4.9 that each of the methods does equally well in approximation of the exponential decay of the motion. In fact, if we look at zoomed in view of Fig. 4.9 as seen in Fig. 4.10 we see that the CIMP method is slightly closer to the exponential decay of the exact solution but the difference is so small that it is insignificant and we can effectively say that the methods are nearly equal in their approximation.

In Fig. 4.11 we look at the rate of the energy dissipation and again consider the function (4.4). It is seen that there is no drift in the rate of dissipation for any of the methods as expected, based on the analytical analysis performed earlier in Chapter 2.

Looking at the approximations for the total energy of the systems we see on the left side of Fig. 4.12 that as expected, the CSV1, CSV2, and CIMP methods appear to perform well in their approximations of the total energy $H(q, p)$ when compared to the exact value. As further verifi-

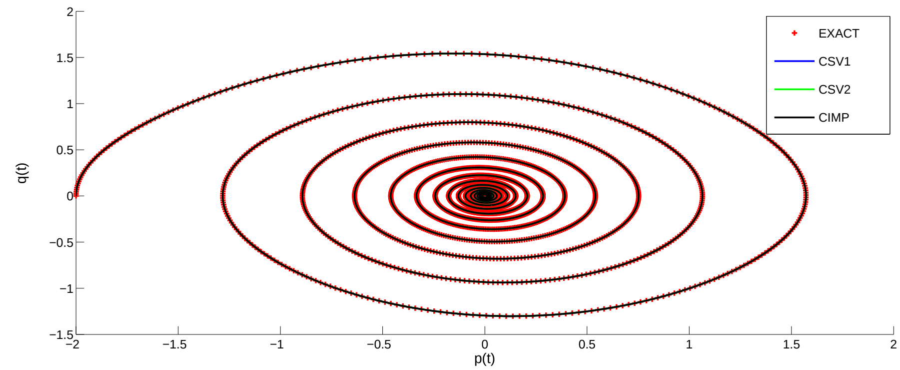

Figure 4.9: Pendulum: Phase space $q(t)$ vs $p(t)$ graph for $\Delta t = .025, \gamma = .05$

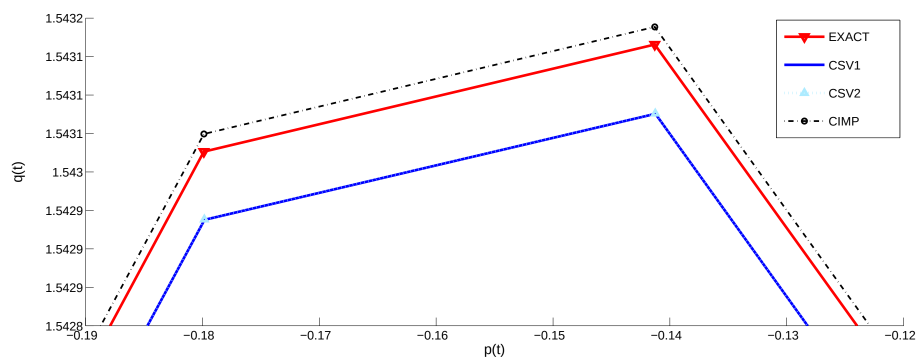

Figure 4.10: Pendulum: Phase space $q(t)$ vs $p(t)$ graph for $\Delta t = .025, \gamma = .05$

cation, we look at the error in the approximations of the total energy by calculating the difference $H_{exact}(q, p) - H_{approx}(q, p)$ and plotting the results as seen in the right side of Fig. 4.12. The difference in total energy graphs on the right side in Fig. 4.12 show the methods to be nearly equal. For further comparison, in Fig. 4.13 we show the total energy difference $H_{exact}(q, p) - H_{approx}(q, p)$ for all the methods together using the same parameters. We find that no one method out performs the other methods in the approximation of the total energy, with each method at some point being slighter superior to the other two. There does appear to be a slightly smaller slope in the error curve of the CIMP method until the point that the damping of the solution has taken affect and the

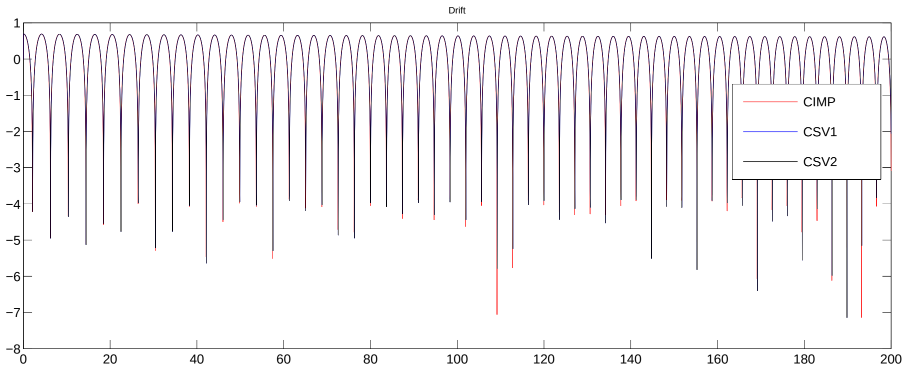

Figure 4.11: Drift in rate of energy dissipation $d(t)$ for $\Delta t = .025, \gamma = .0025$

results are less reliable.

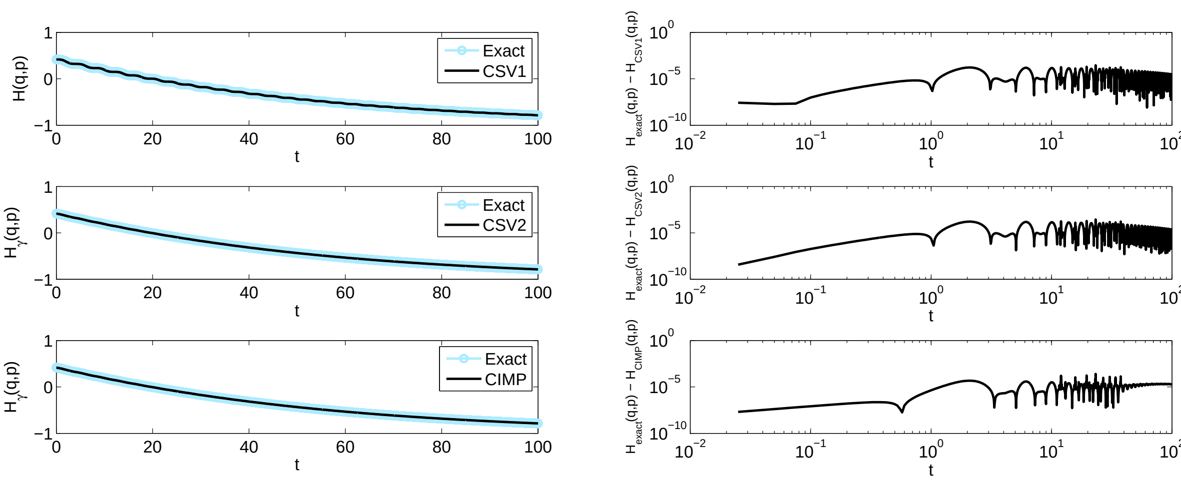

Figure 4.12: Pendulum: Total Energy $H(q, p)$ with $\Delta t = .025, \gamma = .02$

For a final comparison of the methods we show the operational costs. In Table. 4.1 we show, for various values of the damping coefficient γ, the number of function calls for each method. As expected for an implicit method the CIMP method consistently showed a significant increase in the number of function calls when compared to the explicit CSV1 and CSV2 methods.

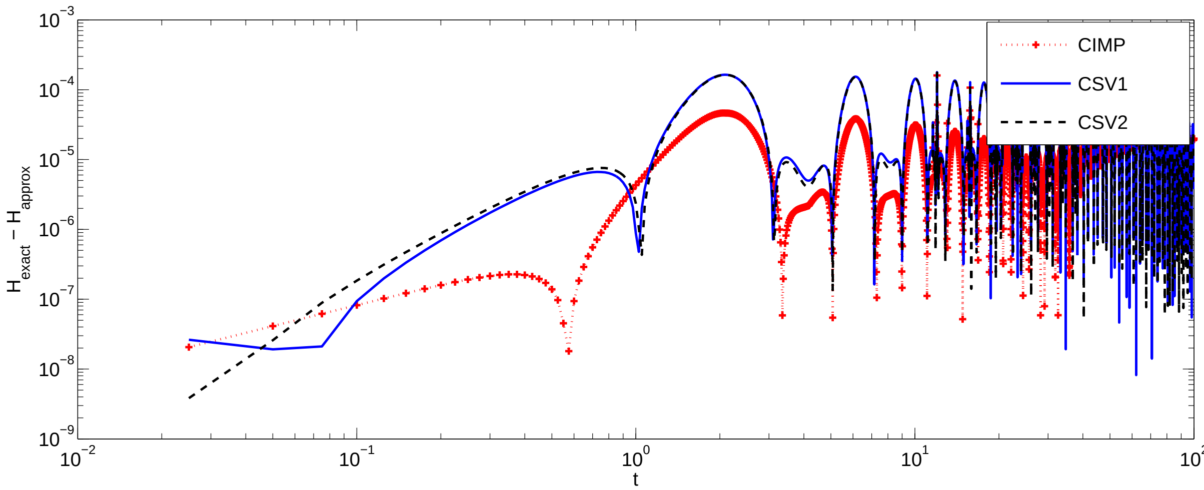

Figure 4.13: Total Energy Error $H_{exact}(q,p) - H_{approx}(q,p)$ with $\Delta t = .025, \gamma = .02$

Table 4.1: Number of function calls varying the damping coefficient γ and $\Delta t = .025$.

γ	0	.00005	.0005	.005	.05	.5
CIMP	15325	15351	15353	14753	14155	11119
CSV1	8000	8000	8000	8000	8000	8000
CSV2	8000	8000	8000	8000	8000	8000

CHAPTER 5: CONCLUSION

Two explicit methods based upon the Störmer-Verlet method and one implicit method based upon the implicit midpoint method were shown to be conformal symplectic integrators and it was proven they each preserved the rate of angular momentum dissipation. Another finding of significance was seen in Fig. 4.7 when the rate of dissipation of the methods was compared to that of a 3rd order Runge-Kutta. In those findings, it was obvious that a clear drift in the rate of dissipation was present in the higher order Runge-Kutta method that was not present in the 2nd order Conformal Störmer-Verlet methods or the 2nd order Conformal Implicit Midpoint method.

An analytical linear stability analysis was completed for each method providing thresholds between the values of the damping coefficient γ and the step-size Δt in order to ensure stability. The importance here, is that an actual relation between the parameters was established instead of relying upon the use of sufficiently small values of the damping coefficient. Verification of the higher computational costs associated with the Conformal Implicit Midpoint method was included in the comparison of the methods.

The analytical and numerical results of thesis show that the Conformal Störmer-Verlet methods and the Conformal Implicit Midpoint methods produce similar results when applied to a damped harmonic oscillator and a damped nonlinear pendulum. Of importance here, is that the two Störmer-Verlet methods are explicit methods and therefore have smaller computational costs than the Conformal Implicit Midpoint method. Given the similarity of the results produced by each of the methods, it would seem within the scope of this thesis that the two explicit Störmer-Verlet methods are an attractive alternative when selecting a numerical method.

A more thorough understanding of these methods could be found by further study using Hamiltonian ODE and PDE systems with linear dissipation that have more practical application. At the very least, it seems apparent that further study into the validity of the results is warranted to see if the results continue to remain consistent across more complex systems of equations.

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