OPERATOR SPLITTING METHODS FOR DIFFERENTIAL EQUATIONS

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Yeşim YAZICI

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İZMİR

We approve the thesis of **Yeşim YAZICI**

Assoc. Prof. Dr. Gamze TANOĞLU
Supervisor

Prof. Dr. Turgut ÖZİŞ
Committee Member

Assoc. Prof. Dr. Ali İhsan NESLİTÜRK
Committee Member

13 May 2010

Prof. Dr. Oğuz YILMAZ
Head of the Department of
Mathematics

Assoc. Prof. Dr. Talat YALÇIN
Dean of the Graduate School of
Engineering and Sciences

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ABSTRACT

OPERATOR SPLITTING METHODS FOR DIFFERENTIAL EQUATIONS

In this thesis, consistency and stability analysis of the traditional operator splitting methods are studied. We concentrate on how to improve the classical operator splitting methods via Zassenhaus product formula. In our approach, acceleration of the initial conditions and weighted polynomial ideas for each cases are individually handled and relevant algorithms are obtained. A new higher order operator splitting methods are proposed by the means of Zassenhaus product formula and rederive the consistency bound for traditional operator splitting methods. For unbounded operators, consistency analysis are proved by the C_0-semigroup approach. We adapted the Von-Neumann stability analysis to operator splitting methods. General approach to use Von-Neumann stability analysis are discussed for the operator splitting methods. The proposed operator splitting methods and traditional operator splitting methods are applied to various ODE and PDE problems.

ÖZET

DİFERANSİYEL DENKLEMLER İÇİN OPERATÖR AYIRMA METODLARI

Bu tezde geleneksel operatör ayırma metodlarının kararlılık ve tutarlılık analizleri çalışılmıştır. Klasik anlamdaki operatör ayırma metodlarının Zassenhaus çarpım formulü ile nasıl geliştirildiğine yoğunlaşılmıştır. Yaklaşımımızda, başlangıç koşullarının akselerasyonu ve ağırlaştırılmış polinom fikri her durum için ayrı ayrı işlenmiş ve ilgili algoritmalar elde edilmiştir. Zassenhaus çarpım formulü ile elde edilen yeni yüksek dereceli operatör ayrıma metodları sunulmuş ve geleneksel operatör ayrıma metodları için tutarlılık sınırları yeniden elde edilmiştir. Sınırsız operatörler için tutarlılık analizleri C_0-yarıgrup yaklaşımı ile yapılmıştır. Von-Neumann kararlılık analizi operatör ayırma metodları için uyarlanmıştır ve geleneksel yaklaşımı tartışılmıştır. Önerilen operatör ayırma metodları ve geleneksel operatör ayırma metodları çeşitli adi ve kısmi diferansiyel denklemler için uygulanmıştır.

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CHAPTER 1

INTRODUCTION

Operator splitting is a powerful method for numerical investigation of complex models. The basic idea of the operator splitting methods based on splitting of complex problem into a sequence of simpler tasks, called split sub-problems. The sub operators are usually chosen with regard to different physical process. Then instead of the original problem, a sequence of sub models are solved, which gives rise to a splitting error. The order of the splitting error can be estimate theoretically. In practice, splitting procedures are associated with different numerical methods for solving the sub-problems, which also causes a certain amount of error.

The idea of operator splitting, which was the Lie-Trotter splitting, dates back to the 1950s. It was probably in 1957 that this method was first used in the solution of partial differential equations (Bagrinovskii & Godunov, 1957). The first splitting methods were developed in the 1960s or 1970s and were based on fundamental results of finite difference methods. The classical splitting methods are the Lie-Trotter splitting, the Strang splitting (Dimov et al., 2001), (Strang, 1968), (Faragó & Havasi, 2007) and the symmetrically weighted splitting (Strang, 1963), (Csomós et al., 2005). A renewal of the methods was done. In the 1980s while using the methods or complex process underlying partial differential methods in (Crandall & Majda, 1999).

Complex physical processes are frequently modelled by the systems of linear or non-linear partial differential equations. Due to the complexity of these equations, typically there is no numerical method which can provide a numerical solution that is accurate enough while taking reasonable integrational time. In order to simplify the task (Strang, 1968), (Marchuk, 1988) operator splitting procedure has been introduced, which is widely used for solving advection-diffusion-reaction problems in (Hvistendahl et al., 2001), (Marinova et al., 2003) Navier-Stokes equation in (Christov & Marinova, 2001), including modelling turbulence (Mimura et al., 1984) and interfaces.

The main idea is to decouple a complex equation in various simpler equations and to solve the simpler equations with adapted discretisation and solver methods. The methods are described in the literature for the basic studies in (Verwer & Sportisse, 1998) and (Strang, 1968).

In many applications in the past, a mixing of various terms in the equations for the discretization and solver methods made it difficult to solve them together. With respect to the adapted methods for a simpler equation, the methods give improved results for simpler parts.

The higher order operator splitting methods are used for more accurate computations, but also with respect to more computational steps. These methods are often performed in quantum dynamics to approximate the evolution operator $exp(\tau(A+B))$. The construction of the higher order methods is based on the forward and backward time step, due to the reversibility. There have been some composition techniques to get the higher order splitting methods. The well known higher order composition schemes are developed by many authers (Blanes & Moan, 2002), (Kahan & Li, 1997), (Mclachlan & Quispel, 2002), (Suzuki, 1990), (Yoshida, 1990).

The consistency of difference splitting schemes has been thoroughly investigated in the terms of the local splitting error (Dimov et al., 2001), (Csomós et al., 2005). These studies are based on the traditional power series expansion of the exact solution and of the solution of the obtained by splitting and recently with semigroup theory for abstract homogenous and non-homogenous Cauchy problem, see in (Bjórhus, 1988). For a special class of unbounded operators, the so-called generators of strongly continuous semigroups (or C_0-semigroups) the Taylor series still have a convenient form. By means of this formula, the consistency analysis of the traditional operator splitting methods have been performed for generators of C_0-semigroups by Bjórhus (Bjórhus, 1988).

The outline of this thesis can be given as follows: Chapter 2 introduces the Lie-Trotter splitting, Strang splitting, symmetrically weighted splitting, additive splitting and higher order splitting. We prove the orders of these methods in terms of the Taylor series expansion. Chapter 3 focuses on the Zassenhaus product formula and relation between the operator splitting methods. In Chapter 4, we study the consistency analysis of the operator splitting methods by means of the Zassenhaus product formula and also with semigroup theory for unbounded operators. In Chapter 5, we discuss the general approach to use the Von-Neumann stability analysis. Von-Neumann stability analysis of proposed algorithms are used to achieve linear stability criteria to model problem, nonlinear KdV equation. In Chapter 6, we give some numerical examples of various ODE and PDE problems with traditional and higher order operator splitting methods to show that the operator splitting methods are efficient. Finally, the conclusion is given in Chapter 7.

CHAPTER 2

OPERATOR SPLITTING METHODS

Operator splitting methods are well known in the field of numerical solution of partial differential equations. The technique is generally used in one of the two ways: It is used in methods in which one splits the differential operator such that each split system only involves derivatives along one of the coordinate axes. Alternatively, it is used as a means to split the differential operator into several parts, where each part represents a particular physical phenomenon, such as convection, diffusion, etc. In either case, the corresponding numerical method is defined as a sequence of solves of each of the split problems. This can lead to very efficient methods, since one can treat each part of the original operator independently.

Operator splitting means the spatial differential operator appearing in the equations is split into a sum of different sub-operators having simpler forms, and the corresponding equations can be solved easier. Operator splitting is an attractive technique for solving coupled systems of partial differential equations, since complex equation system maybe split into simpler parts that are easier to solve. Several operator splitting techniques exists, but we will apply a class of methods often referred as fractional step methods.

We focus our attention on the case of two linear operators. Let us consider the Cauchy problem :

$$\frac{\partial U(t)}{\partial t} = AU(t) \ + \ BU(t), \ \text{with } t \in [0, T], \ U(0) = U_0, \tag{2.1}$$

whereby the initial function U_0 is given and A and B are assumed to be bounded linear operators in the Banach-space $\mathbf{X}$ with $A, B : \mathbf{X} \to \mathbf{X}$. In realistic applications the operators corresponds to physical operators such as convection and diffusion operators.

Splitting methods assume that the mathematical problem can be split into two or more terms. We denote by $U(t) = e^{(A+B)t}U_0$ is the solution at the time t of the differential equation (2.1) with initial value $U(0) = U_0$.

While attractive from a theoretical point of view, the fractional operator splitting methods based on exact flows may not be practically feasible. In particular, the exponential mapping may not be computationally available or too expensive to evaluate exactly.

Thus the flow map exp is often approximated using some numerical method. Some of the choices studied in the literature are regular ODE-based integration of a single component of the vector field. A feature of numerical approximations to the exponential function is that such approximations usually do not satisfy the composition property experienced by the exact flow. Distinguishing the different approaches, methods based on exact flows are commonly known as exponential splitting methods.

Having constructed splitting methods for ordinary differential equations, the question naturally arises of how to construct accurate schemes which may be used with non-small step size. One approach in this direction is the construction of higher order methods for which numerical map Φ_t of (2.1) satisfies,

$$\Phi_t = e^{(A+B)t} + \mathcal{O}(t^{p+1}) \tag{2.2}$$

with the order p being as high as possible. A standard technique for obtaining such methods is to compose Φ_t from more than two exponentials.

As such, a typical non-symmetric composition method often used is

$$\Phi_t = e^{a_m Bt} e^{b_m At} ... e^{a_1 Bt} e^{b_1 At} e^{a_0 Bt} e^{b_0 At} \tag{2.3}$$

and various approach have been suggested for determining conditions on the free parameters $a_0, a_1, ..., a_m$ and $b_0, b_1, ..., b_m$.

Any exponential operator splitting method involving several compositions can be cast into the following form,

$$e^{t(A+B)} = \prod_{i=1}^{m} e^{a_i tA} e^{b_i tB} + \mathcal{O}(t^{m+1}) \tag{2.4}$$

where A, B are noncommutative operators, t is equidistance time step, and $(a_1, a_2, ...)$, $(b_1, b_2, ...)$ are real numbers.

For example Lie-Trotter splitting method for (2.1) can be cast into the general form (2.4) with

$$s = 1, \quad a_1 = 1, \quad b_1 = 1 \quad \text{or} \quad a_1 = 0, \quad a_2 = 1, \quad b_1 = 1, \quad b_2 = 0 \tag{2.5}$$

respectively, that is, the first numerical solution value is given by

$$y_1 = e^{Bt}e^{At}y_0, \quad \text{or} \quad y_1 = e^{At}e^{Bt}y_0 \tag{2.6}$$

Strang splitting method can be cast into the form (2.4) with

$$s = 2, \quad a_1 = a_2 = \frac{1}{2}, \qquad b_1 = 1, \quad b_2 = 0 \tag{2.7}$$

or

$$s = 2, \quad a_1 = 0, \qquad a_2 = 1, \quad b_1 = b_2 = \frac{1}{2} \tag{2.8}$$

respectively, that is, the first numerical solution value is given by

$$y_1 = e^{At/2}e^{Bt}e^{At/2}y_0, \quad \text{or} \quad y_1 = e^{Bt/2}e^{At}e^{Bt/2}y_0 \tag{2.9}$$

In this study, we consider Lie-Trotter splitting and additive splitting as first order splitting methods, Strang splitting and symmetrically weighted splitting as second order splitting methods.

2.1. First Order Splitting: Lie-Trotter Splitting

First, we describe the first order operator splitting method, which is called Lie-Trotter splitting. Lie-Trotter splitting is introduced as a method, which solves two subproblems sequentially on subintervals $[t^n, t^{n+1}]$, where $n = 0, 1, ..., N-1$, $t^0 = 0$ and $t^N = T$. The different subproblems are connected via the initial conditions.

Lie-Trotter Splitting's algorithm is as follows :

$$\frac{\partial u(t)}{\partial t} = Au(t) \text{ with } t \in [t^n, t^{n+1}] \quad \text{and} \quad u(t^n) = u^n_{sp} \tag{2.10}$$

$$\frac{\partial v(t)}{\partial t} = Bv(t) \quad \text{with } t \in [t^n, t^{n+1}] \quad \text{and} \quad v(t^n) = u(t^{n+1}), \tag{2.11}$$

for $n = 0, 1, ..., N-1$ whereby $u^n_{sp} = U_0$ is given from (2.1). The approximated split solution at the point $t = t^{n+1}$ is defined as $u_{sp}^{n+1} = v(t^{n+1})$.

Although it may now seem that we have found an approximate solution after a time interval $2\triangle t$, we have only included parts of the right hand side in each integration step.To see that result $v(\triangle t)$ is in fact a consistent approximation to $U(\triangle t)$ we perform a Taylor series expansion of both the original solution U, and the approximation v obtained by the operator splitting.We have,

$$U(\triangle t) = U_0 + \triangle t \frac{\partial U}{dt} + \frac{\triangle t^2}{2!} \frac{\partial^2 U}{\partial t^2} + \mathcal{O}(\triangle t^3) \tag{2.12}$$

where,

$$\frac{\partial U}{\partial t} = (A + B)U \tag{2.13}$$

and if A and B do not depend explicitly on t, we obtain by direct differentiation

$$\frac{\partial^2 U}{\partial t^2} = (A + B)(A + B)U \tag{2.14}$$

for which we introduce the shorter rotation

$$\frac{\partial^2 U}{\partial t^2} = (A + B)^2 U \tag{2.15}$$

Repeating these steps n times gives the general result,

$$\frac{\partial^n U}{\partial t^n} = (A + B)^n U \tag{2.16}$$

where the notation $(A+B)^n$ simply means that operator $(A+B)$ is applied n times to U. Inserted into the Taylor series, this gives

$$U(\triangle t) = U_0 + \triangle t(A + B)U_0 + \frac{\triangle t^2}{2!}(A + B)^2 U_0 + \mathcal{O}(\triangle t^3) \tag{2.17}$$

A similar Taylor expansion can be made for the solution u of the simplified equation (2.10). We get,

$$u(\triangle t) = U_0 + \triangle t A U_0 + \frac{\triangle t^2}{2!} A^2 U_0 + \mathcal{O}(\triangle t^3) \tag{2.18}$$

We now use the same series expansion for the solution of (2.11), with $u(\triangle t)$ as the initial condition. We get,

$$v(\triangle t) = u(\triangle t) + \triangle t B u(\triangle t) + \frac{\triangle t^2}{2!} B^2 u(\triangle t) + \mathcal{O}(\triangle t^3) \tag{2.19}$$

and inserting the series expansion for $u(\triangle t)$ gives,

$$v(\triangle t) = U_0 + \triangle t(A + B)U_0 + \frac{\triangle t^2}{2!}(A^2 + 2BA + B^2)U_0 + \mathcal{O}(\triangle t^3) \tag{2.20}$$

The splitting error at $t = \triangle t$ is the difference between the operator splitting solution $v(\triangle t)$ and the solution $U(\triangle t)$ of the original problem.Inserting the series expansion (2.17) and (2.20) we get,

$$\frac{v(\triangle t) - U(\triangle t)}{\triangle t} = \frac{\triangle t}{2}[A, B]U_0 + \mathcal{O}(\triangle t^2) \tag{2.21}$$

We see that the error after one time step we expect this error accumulate to n$\triangle t^2$ after n time step. We define $[A, B] := AB - BA$ as the commutator of A and B. Consequently, the splitting error is $\mathcal{O}(\triangle t^2)$. When the operators commute, then the method is exact.

2.2. First Order Splitting: Additive Splitting

This method is based on a simple idea: we solve the different sub-problems by using the same initial function. We obtain the split solution by the use of these results and the initial condition. We consider the problem (2.1), in the computation of split solutions of the two subproblems are added, and the initial condition is subtracted from the sum. In this manner we obtain a splitting method where the different subproblems have no effect on each other. The additive splitting method solves two sub-problems sequentially on sub-intervals $[t^n, t^{n+1}]$, where $n = 0, 1, ..., N-1$, $t^0 = 0$ and $t^N = T$.

The additive splitting algorithm is as follows:

$$\frac{\partial u(t)}{\partial t} = Au(t) \text{ with } t \in [t^n, t^{n+1}] \quad \text{and} \quad u(t^n) = u_{sp}^n \tag{2.22}$$

$$\frac{\partial v(t)}{\partial t} = Bv(t) \quad \text{with } t \in [t^n, t^{n+1}] \quad \text{and} \quad v(t^n) = u_{sp}^n, \tag{2.23}$$

$$u_{sp}^{n+1} = u(t^{n+1}) + v(t^{n+1}) - u_{sp}^n \tag{2.24}$$

for $n = 0, 1, ..., N-1$ whereby $u_{sp}^n = U_0$ is given from (2.1).

To see that additive splitting is a first order accuracy again we use the Taylor expansion of the solutions. Using the series expansion of (2.22) and (2.23) we get,

$$u_{sp}(\triangle t) = U_0 + \triangle t A U_0 + \frac{\triangle t^2 A^2}{2} U_0 + U_0 + \triangle t B U_0 + \frac{\triangle t^2 B^2}{2} U_0 \tag{2.25}$$

$$-U_0 + \mathcal{O}(t^3) \tag{2.26}$$

The splitting error at $t = \triangle t$ is the difference between the operator splitting solution $u_{sp}(\triangle t)$ and the solution $U(\triangle t)$ of the original problem.

$$\frac{u_{sp}(\triangle t) - U(\triangle t)}{\triangle t} = \frac{\triangle t}{2}(BA + AB)U_0 + \mathcal{O}(\triangle t^2) \tag{2.27}$$

We see that additive splitting is a first order method.

2.3. Second Order Splitting: Strang Splitting

One of the most popular and widely used operator splitting method is Strang splitting (or Strang-Marchuk operator splitting method). By the small modification it is possible to make the splitting algorithm second order accurate. The idea is that instead of first solving (2.10) for a full time step length $\triangle t$, we solve the problem for a time step of length $\triangle t/2$. We then solve the problem (2.11) for a full time step of length $\triangle t$, and finally (2.10) once more, again for a time interval of length $\triangle t/2$.

Strang Splitting's algorithm is as follows :

$$\frac{\partial u^*(t)}{\partial t} = Au(t) \text{ with } t \in [t^n, t^{n+1/2}], \quad u(t^n) = u^n_{sp} \tag{2.28}$$
$$\frac{\partial v(t)}{\partial t} = Bv(t) \quad \text{ with } t \in [t^n, t^{n+1}], \quad v(t^n) = u(t^{n+1/2}) \tag{2.29}$$
$$\frac{\partial w(t)}{\partial t} = Aw(t) \text{ with } t \in [t^{n+1/2}, t^{n+1}], \quad w(t^{n+1/2}) = v(t^{n+1}) \tag{2.30}$$

where $t^{n+1/2} = t^n + 0.5\triangle t$, and the approximated split solution at the point $t = t^{n+1}$ is defined as $u^{n+1}_{sp} = w(t^{n+1})$.

In order to show that Strang Splitting gives second order accuracy, we first find a Taylor expansion of the solution u of (2.28), at $t = \triangle t/2$

$$u(\triangle t/2) = U_0 + \frac{\triangle t}{2} AU_0 + \frac{\triangle t^2}{4} A^2 U_0 + \mathcal{O}(\triangle t^3) \tag{2.31}$$

Using this as an initial condition for a Taylor expansion of the solution $v(\triangle t)$ from the second step, we get

$$v(\triangle t) = U_0 + \frac{\triangle t}{2} AU_0 + \triangle t BU_0 + \frac{\triangle t^2}{8} A^2 U_0 + \frac{\triangle t^2}{2} ABU_0 \tag{2.32}$$
$$+ \frac{\triangle t^2}{2} B^2 U_0 + \mathcal{O}(\triangle t^3) \tag{2.33}$$

And finally, by a Taylor expansion of the third step, we find

$$w(\triangle t) = U_0 + \triangle t(A + B)U_0 + \frac{\triangle t^2}{2}(A^2 + AB + BA + B^2)U_0 + \mathcal{O}(\triangle t^3) \tag{2.34}$$

Comparing this with the Taylor expansion (2.12) of the solution (2.1) we get,

$$\frac{w(\triangle t) - U(\triangle t)}{\triangle t} = \mathcal{O}(\triangle t^3) \tag{2.35}$$

and it is seen that Strang splitting gives second order accuracy.

2.4. Second Order Splitting: Symmetrically Weighted Splitting

For noncommuting operators, the Lie-Trotter splitting is not symmetric with respect to the operators A and B, and it has first order accuracy. However in many practical cases we require splittings of higher-order accuracy. We can achieve this by the following modified splitting method, called Symmetrically Weighted Splitting which is already symmetrical with respect to the operators. The sequential operator splitting method solves two sub-problems sequentially on sub-intervals $[t^n, t^{n+1}]$, where $n = 0, 1, ..., N - 1$, $t^0 = 0$ and $t^N = T$.

Symmetrically Weighted Splitting's algorithm is as follows :

$$\frac{\partial u_1(t)}{\partial t} = Au_1(t) \quad , \quad u_1(t^n) = u_{sp}^n \tag{2.36}$$
$$\frac{\partial v_1(t)}{\partial t} = Bv_1(t) \quad , \quad v_1(t^n) = u_1(t^{n+1}) \tag{2.37}$$
$$\frac{\partial u_2(t)}{\partial t} = Bu_2(t) \quad , \quad u_2(t^n) = u_{sp}^n \tag{2.38}$$
$$\frac{\partial v_2(t)}{\partial t} = Av_2(t) \quad , \quad v_2(t^n) = u_2(t^{n+1}), \tag{2.39}$$

for $n = 0, 1, ..., N - 1$ whereby $u_{sp}^n = U_0$ is given from (2.1). Then the approximation at the next time level t^{n+1} is defined as,

$$u_{sp}^{n+1} = \frac{v_1(t^{n+1}) + v_2(t^{n+1})}{2} \tag{2.40}$$

We can easily see that the method is of second order accurate by using the Taylor expansion of the solutions u_1 and u_2 of the simplified equation (2.36) and (2.38).We get,

$$u_1(\triangle t) = U_0 + \triangle t A U_0 + \frac{\triangle t^2}{2!} A^2 U_0 + \mathcal{O}(\triangle t^3) \tag{2.41}$$

We now use the same series expansion for the solution of (2.36), with $u_1(\triangle t)$ as the initial condition. We get,

$$v_1(\triangle t) = u_1(\triangle t) + \triangle t B u_1(\triangle t) + \frac{\triangle t^2}{2!} B^2 u_1(\triangle t) + \mathcal{O}(\triangle t^3) \tag{2.42}$$

and inserting the series expansion for $u_1(\triangle t)$ gives,

$$v_1(\triangle t) = U_0 + \triangle t(A+B)U_0 + \frac{\triangle t^2}{2!}(A^2 + 2BA + B^2)U_0 + \mathcal{O}(\triangle t^3) \tag{2.43}$$

Doing the same for the second part we get,

$$u_2(\triangle t) = U_0 + \triangle t B U_0 + \frac{\triangle t^2}{2!} B^2 U_0 + \mathcal{O}(\triangle t^3) \tag{2.44}$$

We now use the same series expansion for the solution of (2.38), with $u_2(\triangle t)$ as the initial condition. We get,

$$v_2(\triangle t) = u_2(\triangle t) + \triangle t A u_2(\triangle t) + \frac{\triangle t^2}{2!} A^2 u_2(\triangle t) + \mathcal{O}(\triangle t^3) \tag{2.45}$$

and inserting the series expansion for $u_2(\triangle t)$ gives,

$$v_2(\triangle t) = U_0 + \triangle t(A+B)U_0 + \frac{\triangle t^2}{2!}(A^2 + 2BA + B^2)U_0 + \mathcal{O}(\triangle t^3) \tag{2.46}$$

We know that,

$$u_{sp}(\triangle t) = \frac{v_1(\triangle t) + v_2(\triangle t)}{2} \tag{2.47}$$

The splitting error at $t = \triangle t$ is difference between the operator splitting solution $u_{sp}(\triangle t)$ and the solution $U(\triangle t)$ of the original problem.

$$\frac{u_{sp}(\triangle t) - U(\triangle t)}{\triangle t} = \mathcal{O}(\triangle t^3) \tag{2.48}$$

we can easily see that symmetrically weighted splitting is a second order splitting method.

2.5. Higher Order Splitting Method

The higher order operator splitting methods are used for more accurate computations, but also with respect to more computational steps. These methods are often performed in quantum dynamics to approximate the evolution operator $e^{(A+B)t}$.

An analytical construction of higher order splitting methods can be performed with the help of Baker-Campbell-Hausdorff formula, which is proposed initially by J.E. Campbell in 1898 and subsequently proved independently by Baker in 1905 (Baker, 1905) and Hausdorff in 1906. Baker-Campbell-Hausdorff (BCH) formula expresses the product of two exponentials as one new exponential:

$$e^{At}e^{Bt} = e^{\hat{A}t} \tag{2.49}$$

with

$$\hat{A} = (A+B) + \frac{1}{2}t[B,A] + \frac{1}{12}t^2([B,[B,A]] + [A,[A,B]]) \tag{2.50}$$
$$+\frac{1}{24}t^3[B,[A,[A,B]]] + \mathcal{O}(t^4). \tag{2.51}$$

Clearly, if A, B commute all higher-order terms in the expansion vanish and $\hat{A} = A + B$.

The reconstruction process is based on the following product of exponential functions:

$$e^{t(A+B)} = \prod_{i=1}^{m} e^{a_i tA} e^{b_i tB} + \mathcal{O}(t^{m+1}) \tag{2.52}$$

where A, B are noncommutative operators, t is equidistance time step, and $(a_1, a_2, ...)$, $(b_1, b_2, ...)$ are real numbers.

For a fourth order method, we have the following coefficients,

$$a_1 = a_4 = \frac{1}{2(2-2^{1/3})}, \qquad a_2 = a_3 = \frac{1-2^{1/3}}{2(2-2^{1/3})} \tag{2.53}$$
$$b_1 = b_3 = \frac{1}{2-2^{1/3}}, \qquad b_2 = -\frac{2^{2/3}}{2-2^{1/3}}, \quad b_4 = 0 \tag{2.54}$$

Many authers constructed different higher order methods by various composition techniques. Exponential operator splitting methods of order four and six are given in Table 2.1.

Table 2.1. Exponential operator splitting methods of order p involving s compositions.

method	order	comp.
Mclachan	p=2	s=3
Strang	p=2	s=2
Blanes-Moan(BM4-2)	p=4	s=7
Suzuki(S4)	p=4	s=6
Yoshida(Y4)	p=4	s=4
Kahan	p=6	s=10
Suzuki (S6)	p=6	s=26
Yoshida(Y6)	p=6	s=8
Blanes-Moan(BM6-1)	p=6	s=11

CHAPTER 3

HIGHER ORDER OPERATOR SPLITTING METHODS VIA ZASSENHAUS PRODUCT FORMULA

In the previous chapter we showed that any exponential splitting method involving several compositions can be cast into the form (2.4). Similarly, the exponential of the sum of two non-commutative operators A and B may be written as an infinite product as follow,

$$e^{A+B} = e^A e^B \prod_{n=2}^{\infty} e^{D_n} \tag{3.1}$$

which is known as the Zassenhaus product. The Zassenhaus exponents D_n may be also expressed as linear combinations a polynomial representation, and not the desired representation in terms of the nested commutators. In the literature, several different approaches concerning the question how to calculate Zassenhaus exponents can be found. In a number of independent papers, Dynkin (Dynkin, 1947), Specht (Specht, 1948), Wever (Wever, 1947) provided a simple explicit construction of such commutator representation. We use the formal power series expansion of the exponential function and comparison technique to find the Zassenhaus exponents.

We solve the initial value problem (2.1). We assume A and B are bounded and constant operators. From the Zassenhaus product formula we have the form (3.1), Expansion of the left hand side of (3.1) yields,

$$e^{(A+B)t} = I + (A+B)t + \frac{(A+B)^2}{2}t^2 + \mathcal{O}(t^3) \tag{3.2}$$

and right hand side of (3.1) yields,

$$\begin{aligned} e^{At}e^{Bt}e^{D_2t^2}... &= \left(I + At + \frac{A^2t^2}{2}...\right)\left(I + Bt + \frac{B^2t^2}{2}...\right)(I + D_2t^2) + \mathcal{O}(t^3) \\ &= I + (A+B)t + \left(\frac{A^2}{2} + AB + \frac{B^2}{2} + D_2\right)t^2 + \mathcal{O}(t^3) \end{aligned} \tag{3.3}$$

By comparing the (3.2) and (3.3), D_2 can be found as,

$$D_2 = -\frac{1}{2}[A, B]. \tag{3.4}$$

We use the following expansions to find the value of D_3

$$e^{At}e^{Bt} = (I + At + \frac{A^2t^2}{2} + \frac{A^3t^3}{6} + ...)(I + Bt + \frac{B^2t^2}{2} + \frac{B^3t^3}{6} + ...) \tag{3.5}$$

and

$$e^{D_2t^2}e^{D_3t^3} = (I + D_2t^2 + D_3t^3) + \mathcal{O}(t^4) \tag{3.6}$$

The right hand side of (3.1) can be expand as follows,

$$\begin{aligned} e^{At}e^{Bt}e^{D_2t^2}e^{D_3t^3}... &= I + (A+B)t + \left(\frac{A^2}{2} + \frac{B^2}{2} + AB + D_2\right)t^2 \\ &+ \left(\frac{A^3}{6} + \frac{B^3}{6} + \frac{A^2B}{2} + \frac{AB^2}{2} + (A+B)D_2 + D_3\right)t^3 \\ &+ \mathcal{O}(t^4) \end{aligned} \tag{3.7}$$

and the left hand side of (3.1) yields,

$$e^{(A+B)t} = I + (A+B)t + \frac{(A+B)^2}{2}t^2 + \frac{(A+B)^3}{6}t^3 + \mathcal{O}(t^4) \tag{3.8}$$

By comparing the (3.7) and (3.8), D_3 can be found as,

$$D_3 = \frac{1}{6}[A, [A, B]] - \frac{1}{3}[B, [B, A]]. \tag{3.9}$$

Again, using the formal power series expansion of exponential function, we have the following form,

$$
\begin{aligned}
e^{(A+B)t} &= \sum_{k=0}^{\infty} \frac{1}{k!}(A+B)^k t^k = I + (A+B)t \\
&\quad + (\frac{1}{2}A^2 + \frac{1}{2}AB + \frac{1}{2}BA + \frac{1}{2}B^2)t^2 + ... \\
&= (I + \frac{At}{2} + ...)(I + Bt + ...)(I + \frac{At}{2} + ...) \prod_{n=3}^{\infty} (e^{D_n t^n}) \\
&= e^{\frac{At}{2}} e^{B} e^{\frac{At}{2}} e^{D_3 t^3} e^{D_4 t^4} .... \qquad (3.10)
\end{aligned}
$$

Our aim is to compute the polynomials D_3 which is a function of commutators $[., [[.,]]]$. By comparing the exact solution given in (3.10) with the expansion up to the order $\mathcal{O}(t^4)$, given in the following equation,

$$
\begin{aligned}
e^{At/2} e^{Bt} e^{At/2} e^{D_3 t^2} ... &= I + (A+B)t + (\frac{BA + B^2 + AB + A^2}{2})t^2 \\
&\quad + (\frac{BAA}{8} + \frac{BBA}{4} + \frac{A^3}{8} + \frac{ABA}{4})\tau^3 \\
&\quad + (\frac{ABB}{4} + \frac{AAB}{8} + D_3)t^3 + \mathcal{O}(t^4) \qquad (3.11)
\end{aligned}
$$

D_3 can be found as,

$$
D_3 = \frac{1}{24}[A, [A, B]] - \frac{1}{12}[B, [B, A]]. \qquad (3.12)
$$

Our aim is to improve the accuracy and modify the algorithm for better performance. We first simply explain the basic of idea obtaining higher order result by lower order method in the following example, we then carry this approach in order to develop a higher order operator splitting method. Consider the scalar equation:

$$
y'(t) = f(y), \quad y(0) = y_0 \qquad (3.13)
$$

The exact solution near initial condition is given by the Taylor series expansion as follows,

$$y(t) = y_0 + tf(y_0) + \frac{t^2 f'(y_0) f(y_0)}{2!} + ... \tag{3.14}$$

Next, suppose $f(y)$ is a linear function, $f(y) = ay$, we then have

$$y(t) = (1 + at + \frac{a^2t^2}{2!} + ...)y_0. \tag{3.15}$$

Numerical approximation of this problem on the interval $[0, t]$ by lower order explicit Euler Method is

$$y_{approx}(t) = (1 + at)y_0. \tag{3.16}$$

After the initial condition is accelerated as

$$\tilde{y}_0 = (1 + wt^2)y_0, \tag{3.17}$$

the numerical approximation of the problem can be found by this initial condition in a higher order accuracy. Here, the relaxation constant $w = \frac{a^2t^2}{2!}$ can be obtained by comparing the exact and approximate solution given in (3.14) and (3.17), respectively. We then have a second order accuracy in the solution by a first order method,

$$\tilde{y}_{approx}(t) = (1 + at + \frac{a^2t^2}{2!})y_0 \tag{3.18}$$

We exhibit our approach in Figure (3.1). Here, y_0 is given initial condition and $\hat{y}_0$ is accelerated initial condition. By applying low order method to the initial value problem with the initial condition $\hat{y}_0$ yield the higher order result $\hat{y}_{app}(t)$.

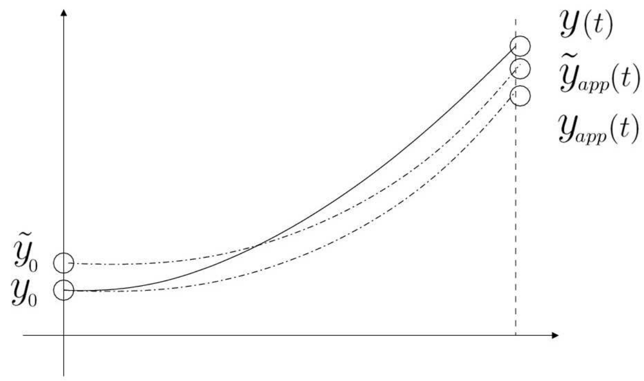

Figure 3.1. By changing initial data, the higher order result can be obtained.

The underlying idea is to improve the initial condition of the splitting schemes. We can shift the approximated solution with the improved initial condition to the exact solution and we obtain (Geiser et al., 2009):

$$||y - \tilde{y}_{approx}|| \leq ||y - y_{approx}||, \tag{3.19}$$

while $\tilde{y}_{approx}$ is approximated by higher order terms.

We focus on the Cauchy problem (2.1) and deal with the following schemes: For the classical Lie-Trotter or A-B splitting, we have globally a first order scheme

$$||(e^{(A+B)t} - e^{At}e^{Bt})U_0|| \leq O(t^2), \tag{3.20}$$

where $e^{(A+B)}t$ is the exact solution given in (2.1) and $e^{At}e^{Bt}$ the approximated solution, t is the local time-step, see (Engel & Nagel, 2000).

For the Strang-Marchuk or A-B-A splitting, we have globally a second order scheme

$$||(e^{(A+B)t} - e^{At/2}e^{Bt}e^{At/2})U_0|| \leq O(t^3), \tag{3.21}$$

where $e^{(A+B)}t$ is the exact solution given in (2.1) and $e^{At/2}e^{Bt}e^{At/2}$ the approximated solution, t is the local time-step, see (Strang, 1968).

In classical operator splitting errors, we have often the problem of improving the lower order methods, see (Sheng, 1993). One helpful method is to improve the initial condition by a weighted function, see Figure (3.1).

We derive a weighted function based on the initial conditions:

$$||U(t) - W(t)U_n|| \leq O(t^m) \tag{3.22}$$

where $U(t)$ is the operator for the classical function, e.g. $W(t) = \exp(At)\exp(Bt)$ for the A-B splitting.

It can be improved by

$$||U(t) - W(t)\tilde{U}_n|| \leq O(t^{m+p}) \tag{3.23}$$

where $\tilde{U}_n = \tilde{W}(t)U_n$ and $\tilde{W}(t)$ is the operator for weighted function, see e.g. Zassenhaus method, (Scholz & Weyrauch, 2006).

3.1. Higher Order Lie-Trotter Splitting by Accelerating the Subproblems Via *Weighted Polynomials*

We gave the algorithm of the Lie-trotter splitting in the previous chapter and showed that the Lie-trotter splitting is a first order method. The order of the method may be increase by the following theorems.

Theorem 3.1 *We solve the initial value problem (2.10), (2.11) on the subinterval [0,t]. We assume bounded and constant operators A and B. The consistency error of the Lie-Trotter splitting is $O(t)$, then we can improve the error of the Lie-Trotter splitting scheme to $O(t^2)$ by multiplied by the initial condition with the weight $w_2 = I + D_2t^2$.*

Proof The splitting error of Lie-Trotter splitting or A-B splitting is

$$\begin{aligned} \rho &= \exp((A+B)t) - \exp(At)\exp(Bt) && (3.24) \\ &= -(\frac{1}{2}[A,B])t^2 && (3.25) \end{aligned}$$

The coefficient of t^2 given in the expansion

$$e^{(A+B)t} = e^{At}e^{Bt}e^{D_2 t^2} + \mathcal{O}(t^3) \tag{3.26}$$

is

$$D_2 + \frac{(A+B)^2}{2!} - \rho,$$

thus, if we choose $D_2 = \rho$, the splitting error becomes $\mathcal{O}(t^3)$. □

Theorem 3.2 *We solve the initial value problem (2.10) and (2.11) on the subinterval [0,t]. The consistency error of the A-B splitting is $\mathcal{O}(t)$, then we can improve the error of the A-B splitting scheme to $\mathcal{O}(t^p)$, $p > 1$ by improving the starting conditions U_0 as*

$$U_0 = (\prod_{j=2}^{p} \exp(D_j t^j))U_0$$

where D_j is called as Zassenhaus exponents, thus local splitting error of A-B splitting method can be read as follows:

$$\begin{aligned} \rho &= (\exp(t(A+B)) - \exp(tB)\exp(tA))u_{sp} \\ &= D_T \; t^{p+1} + \mathcal{O}(t^{p+2}) \end{aligned} \tag{3.27}$$

where D_T is a function of Lie brackets of A and B.

Proof Let us consider the subinterval [0, t], where t is time step size, the solution of the subproblem (2.10) is:

$$u(t) = \exp(At)U_0 \tag{3.28}$$

after improving the initialization we have

$$u(t) = \exp(At)(\prod_{j=2}^{p}\exp(D_j t^j))U_0 \qquad (3.29)$$

the solution of the subproblem (2.11) becomes

$$\begin{aligned} v(t) &= \exp(Bt)\,\exp(At)(\prod_{j=2}^{p}\exp(D_j t^j))U_0 \qquad (3.30)\\ &= \exp((B+A)t)U_0 + \mathcal{O}(t^{p+1}) \end{aligned}$$

□

3.2. Higher Order Strang Splitting by Accelerating the Subproblems Via *Weighted Polynomials*

In order to obtain higher order Strang splitting, we present the idea of the *Weighted Polynomials* in the following theorem:

Theorem 3.3 *We solve the initial value problem (2.28), (2.29) and (2.30) on the subinterval [0,t]. We assume bounded and constant operators A and B. The consistency error of the Strang splitting is $O(t^2)$, then we can improve the error of the Strang splitting scheme to $O(t^3)$ by multiplied by the initial condition with the weight $w_3 = I + D_3 t^3$.*

Proof The splitting error of Strang splitting or A-B-A splitting is

$$\begin{aligned} \rho &= \exp((A+B)t) - \exp(At/2)\exp(Bt)\exp(At/2) \qquad (3.31)\\ &= (\frac{1}{24}[B,[B,A]] - \frac{1}{12}[A,[A,B]])t^3 \qquad (3.32) \end{aligned}$$

The coefficient of t^3 given in the expansion

$$e^{(A+B)t} = e^{\frac{At}{2}}e^{B}e^{\frac{At}{2}}e^{D_3 t^3} + \mathcal{O}(t^4) \qquad (3.33)$$

is

$$D_3 + \frac{(A+B)^3}{3!} - \rho, \tag{3.34}$$

thus, if we choose $D_3 = \rho$, the splitting error becomes $\mathcal{O}(t^3)$. $\square$

Theorem 3.4 *We solve the initial value problem (2.28), (2.29) and (2.30) on the subinterval [0,t]. We assume bounded and constant operators A and B. The consistency error of the Strang splitting is $O(t^2)$, then we can improve the error of the Strang splitting scheme to $O(t^p), p > 2$ by applying the following steps:*

- *Step 1: Improve the starting conditions $u(0) = U_0$ as*

$$u(0) = (\prod_{j=2}^{p} \exp(D_j t^j))U_0$$

where D_j is called as Zassenhaus exponents,

- *Step 2 : Accelerate $v(0)$ as*

$$v(0) = e^{-At}u(t/2),$$

- *Step 3: Accelerate $w(t/2)$ as*

$$w(t/2) = e^{At/2}v(t),$$

thus the order of the A-B-A splitting method can be read as follows

$$e^{(At)/2}e^{Bt}e^{(At)/2} = e^{(A+B)t} + \mathcal{O}(t^{p+1}). \tag{3.35}$$

Proof Let us consider the subinterval [0, t], the solution of the subproblem (2.28) is:

$$u(t) \quad = \quad e^{At}U_0 \tag{3.36}$$

after improving the initialization we have

$$u(t) \quad = \quad e^{At}(\prod_{j=2}^{p} \exp(D_j t^j))U_0. \tag{3.37}$$

Next accelerate $u(t)$ as

$$u(t) \quad = \quad e^{-At} u(t) \tag{3.38}$$

the solution of the subproblem (2.29) becomes

$$\begin{aligned} v(t) \quad &= \quad e^{Bt} u(t/2) && (3.39) \\ &= \quad e^{Bt} e^{-At/2} e^{At/2} (\prod_{j=2}^{p} \exp(D_j (t/2)^j))U_0 && (3.40) \end{aligned}$$

or

$$v(t) \quad = \quad e^{Bt}(\prod_{j=2}^{p} \exp(D_j (t/2)^j))U_0 \tag{3.41}$$

since [-A/2, A/2]=0. Finally, the acceleration of $v(t)$ is given by the equation

$$v(t) \quad = \quad e^{At/2} e^{Bt}(\prod_{j=2}^{p} \exp(D_j (t/2)^j))U_0, \tag{3.42}$$

then the solution of the subproblem (2.29) becomes

$$w(t) \quad = \quad e^{At/2} e^{At/2} e^{Bt}(\prod_{j=2}^{p} \exp(D_j (t/2)^j))U_0 \tag{3.43}$$

or

$$w(t) = e^{At}e^{Bt}(\prod_{j=2}^{p}\exp(D_j(t/2)^j))U_0 \quad (3.44)$$

since [A/2, A/2]=0. This can be rewritten as

$$w(t) = e^{At}e^{Bt}(\prod_{j=2}^{p}\exp(\tilde{D}_j(t)^j))U_0 \quad (3.45)$$

$$= \exp((A+B)t) + \mathcal{O}(t^{p+1}). \quad (3.46)$$

where $\tilde{D}_p = \frac{1}{2^p}D_j$ with the help of the Zassenhaus product formula. □

CHAPTER 4

CONSISTENCY ANALYSIS OF THE OPERATOR SPLITTING METHODS

In the previous chapter, we obtained modified Lie-Trotter and Strang splitting methods by accelerating the initial condition with via Zassenhaus product formula. In this chapter we will obtain the errors for the operator splitting by using Zassenhaus product formula for bounded operators and prove the the consistency of operator splitting methods for unbounded operators by using C_0-semigroup approach.

4.1. Consistency Analysis of the Operator Splitting Methods Based on Zassenhaus Product Formula

In this section, we analyze the consistency and the order of the operator splitting methods by the means of the Zassenhaus product formula. We consider the Cauchy problem (2.1) for linear bounded operators A and B.

The exact solution of (2.1) is given by

$$U(t) = e^{(A+B)t}U_0, \quad t \geq 0. \tag{4.1}$$

As the exact solution operator E_{A+B} is linear with respect to the initial value, we write

$$U(t) = E_{A+B}(h)U_0 = e^{(A+B)t}U_0, \quad t \geq 0. \tag{4.2}$$

Let us divide the time interval $[0, T]$ of the problem into N subintervals of equal length $h = t_{n+1} - t_n$, $n = 0, 1, ..., N-1$ the approximate solution U^{n+1} of $U(t_{n+1})$ is computed as $U^{n+1} = \Phi_{A+B}(h)U^n$ where, Φ_{A+B} is the split solution operator.

In connection with the consistency of a splitting we give the definition of the consistency.

Definition 4.1 *The splitting method is called consistent of order p on $[0, T]$ if,*

$$\lim_{h \to 0} \sup_{0 \le t_n \le T-h} \frac{\|E_{A+B}(h)U(t) - \Phi_{A+B}(h)U(t)\|}{h} = 0 \tag{4.3}$$

and

$$\rho_h = \sup_{0 \le t_n \le T-h} \frac{\|E_{A+B}(h)U(t) - \Phi_{A+B}(h)U(t)\|}{h} = \mathcal{O}(h^p), \quad p > 0, \tag{4.4}$$

4.1.1. Consistency of the Lie-Trotter Splitting Based on Zassenhaus Product Formula

Here we will analyze the consistency and the order of the Lie-Trotter splitting by the means of Zassenhaus product formula for the linear bounded operators A and B in the Banach-space $\mathbf{X}$ with $A, B : \mathbf{X} \to \mathbf{X}$.

Theorem 4.1 *Let A and B be given linear bounded operators. We consider the abstract Cauchy problem (2.1). Lie-Trotter splitting is consistent with the order of $\mathcal{O}(t)$.*

Proof From the Zassenhaus product formula we have the form,

$$e^{(A+B)t} = e^{At} e^{Bt} e^{D_2 t^2} e^{D_3 t^3} \ldots, \tag{4.5}$$

where,

$$D_2 = -\frac{1}{2}[A, B] \tag{4.6}$$

$$D_3 = \frac{1}{6}[A, [A, B]] - \frac{1}{3}[B, [B, A]] \tag{4.7}$$

For the term $e^{D_2t^2}e^{D_3t^3}$ by using the series expansion we can write,

$$\begin{aligned} e^{D_2t^2}e^{D_3t^3} &= (I + D_2t^2 + \mathcal{O}(t^3))(I + D_3t^3 + \mathcal{O}(t^4)) && (4.8) \\ &= I + D_2t^2 + D_3t^3 + \mathcal{O}(t^4) && (4.9) \end{aligned}$$

We can write the equation (4.5) as follows,

$$e^{(A+B)t} = e^{At}e^{Bt} + e^{At}e^{Bt}(I + D_2t^2 + D_3t^3 + \mathcal{O}(t^4)) \quad (4.10)$$

Subtracting the term $e^{At}e^{Bt}$ from the both sides of the equation (4.10) we get,

$$\begin{aligned} e^{(A+B)t} - e^{At}e^{Bt} &= e^{At}e^{Bt}(D_2t^2 + D_3t^3)... && (4.11) \\ &= D_2t^2 + (D_3 + (A+B)D_2)t^3 + \mathcal{O}(t^4) && (4.12) \end{aligned}$$

For Lie-trotter splitting we get

$$e^{(A+B)t} - e^{At}e^{Bt} = -\frac{1}{2}t^2[A, B] + \mathcal{O}(t^3) \quad (4.13)$$

The splitting error of this operator splitting method is derived as follows:

$$\rho_t = \frac{1}{t}(e^{t(A+B)} - e^{At}e^{Bt})U(t) \quad (4.14)$$

The local truncation is found to satisfy,

$$\rho_t = -\frac{1}{2}t[A, B]U_0 + \mathcal{O}(t^2), \quad (4.15)$$

□

4.1.2. Consistency of the Symmetrically Weighted Splitting Based on Zassenhaus Product Formula

Theorem 4.2 *Let, A and B be given linear bounded operators. We consider the abstract Cauchy problem (2.1). Symmetrically weighted splitting is consistent with the order of $\mathcal{O}(t^2)$.*

Proof First we define,

$$\frac{1}{2}e^{(A+B)t} = \frac{1}{2}e^{At}e^{Bt}e^{E_2t^2}e^{E_3t^3}... \quad (4.16)$$
$$\frac{1}{2}e^{(B+A)t} = \frac{1}{2}e^{Bt}e^{At}e^{\tilde{E}_2t^2}e^{\tilde{E}_3t^3}... \quad (4.17)$$

where,

$$E_2 = -\frac{1}{2}[A,B] \quad (4.18)$$
$$\tilde{E}_2 = -E_2 \quad (4.19)$$
$$E_3 = \frac{1}{6}[A,[A,B]] - \frac{1}{3}[B,[B,A]] \quad (4.20)$$
$$\tilde{E}_3 = \frac{1}{6}[B,[B,A]] - \frac{1}{3}[A,[A,B]] \quad (4.21)$$

We get the following by subtracting the summation of equations (4.16) and (4.17) from the term $e^{(A+B)t}$,

$$\begin{aligned}(e^{(A+B)t} - \frac{1}{2}(e^{At}e^{Bt} + e^{Bt}e^{At})) &= \frac{1}{2}(I + (A+B)t)(E_2t^2 + E_3t^3) \\ &\quad + \frac{1}{2}(I + (A+B)t)(\tilde{E}_2t^2 + \tilde{E}_3t^3) \\ &\quad + \mathcal{O}(t^4) \end{aligned} \quad (4.22)$$

Since $E_2 = -\tilde{E}_2$ we have,

$$(e^{(A+B)t} - \frac{1}{2}(e^{At}e^{Bt} + e^{Bt}e^{At})) = \frac{1}{2}(E_3 + \tilde{E}_3) + \mathcal{O}(t^4) \quad (4.23)$$
$$(4.24)$$

where,

$$\frac{1}{2}(E_3 + \tilde{E}_3) = -\frac{1}{12}([A,[A,B]] + [B,[B,A]]) \quad (4.25)$$

The truncation error is,

$$\rho_t = -\frac{1}{12}t^2([A,[A,B]] + [B,[B,A]])U_0 + \mathcal{O}(t^3) \quad (4.26)$$

□

4.1.3. Consistency of the Strang Splitting Based on Zassenhaus Product Formula

Theorem 4.3 *Let, A and B be given linear bounded operators. We consider the abstract Cauchy problem (2.1). Strang splitting is consistent with the order of $\mathcal{O}(t^2)$.*

Proof The exact solution of the (2.1)can be rewritten as follows,

$$e^{(A+B)t} = e^{(A+B)t/2+(B+A)t/2} \quad (4.27)$$

$$= e^{(A+B)t/2}e^{(B+A)t/2} \quad (4.28)$$

Our aim is to show that the consistency error of the Strang Splitting by using Zassenhaus product formula. Let us consider ,

$$e^{(A+B)t/2} = e^{At/2}e^{Bt/2}e^{F_2t^2}e^{F_3t^3}\ldots \quad (4.29)$$

$$e^{(B+A)t/2} = e^{Bt/2}e^{At/2}e^{\tilde{F}_2t^2}e^{\tilde{F}_3t^3}\ldots \quad (4.30)$$

where,

$$F_2 = -\frac{1}{2}\left[\frac{A}{2},\frac{B}{2}\right] \quad (4.31)$$

$$\tilde{F}_2 = -F_2 \quad (4.32)$$

$$F_3 = \frac{1}{6}\left[\frac{A}{2}, \left[\frac{A}{2}, \frac{B}{2}\right]\right] - \frac{1}{3}\left[\frac{B}{2}, \left[\frac{B}{2}, \frac{A}{2}\right]\right] \tag{4.33}$$

$$\tilde{F_3} = \frac{1}{6}\left[\frac{B}{2}, \left[\frac{B}{2}, \frac{A}{2}\right]\right] - \frac{1}{3}\left[\frac{A}{2}, \left[\frac{A}{2}, \frac{B}{2}\right]\right] \tag{4.34}$$

By a series expansion we get,

$$e^{(A+B)t/2} = e^{At/2}e^{Bt/2}(I + F_2t^2 + F_3t^3 + \mathcal{O}(t^4)) \tag{4.35}$$

$$e^{(B+A)t/2} = e^{Bt/2}e^{At/2}(I + \tilde{F}_2t^2 + \tilde{F}_3t^3 + \mathcal{O}(t^4)) \tag{4.36}$$

and we have,

$$\begin{aligned} e^{(A+B)t/2} &= e^{At/2}e^{Bt/2} \\ &\quad + e^{At/2}e^{Bt/2}(F_2t^2 + F_3t^3 + \mathcal{O}(t^4)) \end{aligned} \tag{4.37}$$

$$\begin{aligned} e^{(B+A)t/2} &= e^{Bt/2}e^{At/2} \\ &\quad + e^{Bt/2}e^{At/2}(\tilde{F}_2t^2 + \tilde{F}_3t^3 + \mathcal{O}(t^4)) \end{aligned} \tag{4.38}$$

Multiplying the equations (4.37) and (4.38) we get,

$$\begin{aligned} e^{(A+B)t} &= e^{At/2}e^{Bt/2}e^{Bt/2}e^{At/2} \\ &\quad + e^{At/2}e^{Bt/2}e^{Bt/2}e^{At/2}(\tilde{F}_2t^2 + F_3t^3) \\ &\quad + e^{At/2}e^{Bt/2}(F_2t^2 + F_3t^3)e^{Bt/2}e^{At/2} \\ &\quad + \mathcal{O}(t^4) \end{aligned} \tag{4.39}$$

Using the series expansion,

$$e^{At/2}e^{Bt/2} = (I + \frac{At}{2} + \frac{A^2t^2}{8} + ...)(I + \frac{Bt}{2} + \frac{B^2t^2}{8} + ...) \tag{4.40}$$

$$= I + \frac{(A+B)t}{2} + \mathcal{O}(t^2) \tag{4.41}$$

After some calculations equation (4.39) can be written in the following form,

$$\begin{aligned}(e^{(A+B)t} - e^{At/2}e^{Bt}e^{At/2}) &= ((A+B)\tilde{F}_2 + \frac{(A+B)}{2}F_2 + F_2\frac{(A+B)}{2} \\ &\quad +(F_3 + \tilde{F}_3))t^3 + \mathcal{O}(t^4) \qquad (4.42)\end{aligned}$$

The local truncation error is,

$$\rho_t = \frac{1}{24}t^2([A,[A,B]] - 2[B,[B,A]])U_0 + \mathcal{O}(t^3) \qquad (4.43)$$

□

4.2. Consistency Analysis of Operator Splitting Methods for C_0 Semigroups

The consistency of the operator splitting methods is studied in the previous section for bounded operators by means of the Zassenhaus product formula.In this section, first we introduce the semigroup theory by giving the basic definitions, then rederive the consistency analysis for Lie-Trotter, symmetrically Weighted and Strang Splitting for unbounded generators of strongly continuous semigroup.

4.2.1. Semigroup Theory

Semigroup theory is developed to solve operator ODE. Consider the following linear equation system in ODE

$$\frac{\partial u(t)}{\partial t} = Au(t) \qquad (4.44)$$

$$u(0) = u_0 \qquad (4.45)$$

where the A is matrix of constant coefficient and u is a vector function of time. It is well-known, the solution is $u(t) = e^{At}u(0)$. If A is a linear bounded operator in Banach space, $u(t)$ still has this form. However, in many interesting cases, it is unbounded which don't admit this form. This to some extend shows the richness of semigroup theory.

For its application, semigroup theory uses abstract methods of operator theory to treat initial boundary value problems for linear and nonlinear equations that describe the evolution of a system.

Definition 4.2 *A one-parameter semigroup of operators over a real or complex Banach space* $\mathbf{X}$ *is a family of bounded operators* $S(t)$*,* $t \geq 0$ *satisfy:* $S(t+s) = S(t)S(s)$ *for all t;* $s \geq 0$ *and* $S(0) = I$*.*

1. *A semigroup in* $\mathbf{X}$*,* $\{S(t)\}_{t\geq 0}$*, is called uniformly continuous if* $\lim_{t\to 0^+} S(t) = I$*, where the limit is in the topology of* $S(\mathbf{X})$*.*
2. *A semigroup in* $\mathbf{X}$*,* $\{S(t)\}_{t\geq 0}$*, is called strongly continuous, or* C_0 *for short, if for every* $x \in \mathbf{X}$*,* $\lim_{t\to 0^+} S(t)x = x$*.*
3. *A semigroup in* $\mathbf{X}$*,* $\{S(t)\}_{t\geq 0}$*, is called semigroup of contractions if,*

   $\|S(t)\| \leq 1$ *for every* $t \geq 0$*.*

Observe that in the case of a finite dimensional space, a known example of semigroups are exponentials,

$$S(t) = e^{At} \tag{4.46}$$

Also, observe that once $S(t)$ is known, the matrix A can be determined by,

$$A = \frac{\partial S(t)}{\partial t}, \quad \text{for} \quad t = 0 \tag{4.47}$$

In general case, assume $u(t)$ is solution of (4.44), so $u(t) = S(t)u_0$. Then, if $u_0 \in D(A)$ using (4.44) we must have,

$$u_t(0) = Au_0 \tag{4.48}$$

and left hand side can be written as,

$$u_t(0) = \lim_{t\to 0^+} \frac{S(t)u_0 - u_0}{t} \tag{4.49}$$

This motivates the following definition,

Definition 4.3 *The infinitesimal generator of a C_0 semigroup is the linear operator $(A, D(A))$, whose domain is given by the elements of $\mathbf{X}$ such that,*

$$Ax = \lim_{t \to 0^+} \frac{S(t)x - x}{t} \tag{4.50}$$

exists.

Consider the linear abstract Cauchy problem (4.44)-(4.45) where $A : \mathbf{X} \to \mathbf{X}$ is a closed, densely defined linear operator.Assume that A generates C_0-semigroup $\{S(t)\}_{t \geq 0}$. Then there exist constants $w_0 \in \mathbf{R}$ and $M_0 \geq 1$ such that,

$$\|S(t)\| \leq M_0 e^{w_0 t}, \qquad t \geq 0 \tag{4.51}$$

Moreover, for any $u_0 \in D(A)$ (4.44) has the unique solution

$$u(t) = S(t)u_0, \quad t \geq 0. \tag{4.52}$$

Assume that,

$$A = A_1 + A_2, \tag{4.53}$$

where A_1 and A_2 are generators of such C_0-semigroups $\{S_1(t)\}_{t \geq 0}$ and $\{S_2(t)\}_{t \geq 0}$, which can be approximated more easily than $\{S(t)\}_{t \geq 0}$, respectively satisfying,

$$D(A^k) = D(A_1^k) = D(A_2^k) \quad k = 1, 2, 3 \tag{4.54}$$

Let us divide the time interval $(0, T]$ of the problem into N sub-intervals of equal length $h = t_{n+1} - t_n$. The approximate solution U_s^{n+1} of $u(t_n + 1)$ is compute as,

$$U_s^{n+1} = S_{spl}(h) U_s^n, \tag{4.55}$$

We will concentrate on the following splitting schemes:

1. Lie-Trotter Splitting : $S_{spl}(h) = S_{lie}(h) = S_2(h)S_1(h)$,

2. SWS : $S_{spl}(h) = S_{sym}(h) = \frac{1}{2}(S_2(h)S_1(h) + S_1(h)S_2(h))$,

3. Strang Splitting : $S_{spl}(h) = S_{str}(h) = S_1(h/2)S_2(h)S_1(h/2)$.

Corresponding operator splitting method is consistent in the usual sense:

Define $T_h : \mathbf{X} \times [0, T-h] \to \mathbf{X}$ by

$$T_h(u_0, t) = S(h)u(t) - S_{spl}(h)(h)u(t) \tag{4.56}$$

where $u(t)$ is given by (4.52). Thus for each u_0 and t, $T_h(u_0, t)$ yields the *local truncation error* of the corresponding splitting method.

Definition 4.4 *The splitting method is said to be consistent on* $[0, T]$ *if*

$$\lim_{h\to 0} \sup_{0\le t_n\le T-h} \frac{\|T_h(u_0, t_n)\|}{h} = 0 \tag{4.57}$$

whenever $u_0 \in \mathcal{B}$*,* $\mathcal{B}$ *being some dense subspace of* $\mathbf{X}$.

Definition 4.5 *If in the consistency relation (4.57) we have*

$$\sup_{0\le t_n\le T-h} \frac{\|T_h(u_0, t_n)\|}{h} = \mathcal{O}(h^p), \quad p > 0, \tag{4.58}$$

then the method is said to be (consistent) of order p

The following formula and lemmas will play a basic role in our investigations.

Theorem 4.4 *For any* C_0*-semigroups* $\{S(t)\}_{t\ge 0}$ *of bounded linear operators with corresponding infinitesimal generator* A*, we have the Taylor series expansion*

$$S(t)x = \sum_{j=0}^{n-1} \frac{t^j}{j!}A^j x + \frac{1}{(n-1)!}\int_0^t (t-s)^{n-1} S(s)A^n x ds, \quad \textit{for all } x \in D(A^n) \tag{4.59}$$

Particularly, for $n = 3, 2$ and 1 we get the relations,

$$\begin{aligned} S(h)x &= x + hAx + \frac{h^2}{2}A^2x + \frac{1}{2}\int_0^h (h-s)^2 S(s)A^3 x ds, && (4.60) \\ S(h)x &= x + hAx + \int_0^h (h-s)S(s)A^2 x ds, && (4.61) \\ S(h)x &= x + \int_0^h S(s)Axds, && (4.62) \end{aligned}$$

Lemma 4.1 *Let A and B be closed linear operators from $D(A) \subset \mathbf{X}$ and $D(B) \subset \mathbf{X}$, respectively, into $\mathbf{X}$. If $D(A) \subset D(B)$, then there exists a constant $\hat{\mathcal{C}}$ such that*

$$\|Bx\| \leq \hat{\mathcal{C}}(\|Ax\| + \|x\|) \quad \textit{for all} \quad x \in D(A). \tag{4.63}$$

This implies that there exists a universal constant $\hat{\mathcal{C}}$ by which of $x \in D_k$, $k = 1, 2, 3$

$$\|A_i^k x\| \leq \hat{\mathcal{C}}(\|A_j^k x\| + \|x\|) \quad i, j = 1, 2. \tag{4.64}$$

where,

$$D_k = D(A_1^k) \bigcap D(A_2^k) \bigcap D(A^k) \quad k = 1, 2, 3 \quad \text{dense in} \quad \mathbf{X} \tag{4.65}$$

Lemma 4.2 *Let A be an infinitesimal generator of a C_0-semigroup $\{S(t)\}_{t \geq 0}$. Let $T > 0$ and $n \in \mathbb{N}$ arbitrary. If $u_0 \in D(A^n)$, then $u(t) = S(t)u_0 \in D(A^n)$ for $0 \leq t \leq T$, and we have*

$$\sup_{[0,T]} \|A^k u(t)\| \leq C_k(T), \quad k = 0, 1, ..., n \tag{4.66}$$

where $C_k(T)$ are constants independent of h.

Proof Let $z(t) = A^{n-1}u(t) = A^{n-1}S(t)u_0 = S(t)A^{n-1}u_0$. Clearly, $u_0 \in D(A^n)$

implies $A^{n-1}u_0 \in D(A)$. It is known from the theory of C_0-semigroups [6] that then $S(t)A^{n-1}u_0 \in D(A)$, i.e., $A^{n-1}u(t) \in D(A)$. Consequently, $u(t) \in D(A^n)$. Moreover,

$$\sup_{[0,T]} \|A^k u(t)\| = \sup_{[0,T]} \|A^k S(t)u_0\| = \sup_{[0,T]} \|S(t)A^k u_0\| \leq Me^{|w|T}\|A^k u_0\| \qquad (4.67)$$

for $k = 0, 1, ..., n$ □

4.2.2. Consistency of the Lie-Trotter Splitting

We need to show that the first order consistency of Lie-Trotter Splitting for C_0-semigroups. By using (4.59) for $n = 2$, for $x \in D(A^2)$ we then have,

$$S_2(h)S_1(h)x = S_1(h)x + hA_2S_1(h)x + \int_0^h (h-s)S_2(s)A_2^2S_1(h)xds \qquad (4.68)$$

Substituting

$$S_1(h)x = x + hA_1x + \int_0^h (h-s)S_1(s)A_1^2xds, \qquad (4.69)$$

and

$$S_1(h)x = x + \int_0^h S_1(s)A_1xds, \qquad (4.70)$$

into the first and second terms on the right-hand side of (4.68), respectively, we get

$$S_2(h)S_1(h)x \quad = \quad x + h(A_1x + A_2x) + \int_0^h (h-s)S_1(s)A_1^2xds \qquad (4.71)$$

$$+hA_2 \int_0^h S_1(s)A_1xds \tag{4.72}$$

$$+ \int_0^h (h-s)S_2(s)A_2^2S_1(h)xds \tag{4.73}$$

On the other hand, we have

$$S(h)x = x + hAx + \int_0^h (h-s)S(s)A^2xds, \tag{4.74}$$

so the difference is

$$\begin{aligned} S_2(h)S_1(h)x - S(h)x &= \int_0^h (h-s)S_1(s)A_1^2xds && (4.75)\\ &\quad +hA_2 \int_0^h S_1(s)A_1xds && (4.76)\\ &\quad + \int_0^h (h-s)S_2(s)A_2^2S_1(h)xds && (4.77)\\ &\quad - \int_0^h (h-s)S(s)A^2xds && (4.78) \end{aligned}$$

Proposition 4.1 *Let A, A_1 and A_2 be infinitesimal generators of the C_0-semigroups $\{S(t)\}_{t\geq 0}$, $\{S_1(t)\}_{t\geq 0}$ and $\{S_2(t)\}_{t\geq 0}$, respectively,. Assume that (4.53) and (4.54) are satisfied, and let $T > 0$. Then for all $x \in D$ the relation*

$$\|S_2(h)S_1(h)x - S(h)x\| \leq h^2C(T)(\|A^2x\| + \|Ax\| + \|x\|) \tag{4.79}$$

holds $h \in [0, T]$, where $C(T)$ is a constant of independent of h.

Proof We estimate the terms on the right-hand side of (4.75)-(4.78). The two terms in (4.75) and (4.78) can be estimated directly by

$$\left\| \int_0^h (h-s)S_1(s)A_1^2 x ds \right\| \leq M_1 e^{|w_1|h} \|A_1^2 x\| \frac{h^2}{2} \tag{4.80}$$

and

$$\left\| \int_0^h (h-s)S(s)A^2 x ds \right\| \leq M e^{|w|h} \|A^2 x\| \frac{h^2}{2} \tag{4.81}$$

The term in (4.77) is estimated by

$$\left\| \int_0^h (h-s)S_2(s)A_2^2 S_1(h) x ds \right\| \leq M_2 e^{|w_2|h} \|A_2^2 S_1(h) x\| \frac{h^2}{2}, \tag{4.82}$$

but if we apply (Lemma 4.1) to compare the closed operators A_2^2 and A_1^2 we have,

$$\|A_2^2 S_1(h)x\| \leq \hat{C}(\|A_1^2 S_1(h)x\| + \|S_1(h)x\|), \tag{4.83}$$

which since A_1^2 and $S_1(h)$ commute, yields the estimate

$$\left\| \int_0^h (h-s)S_2(s)A_2^2 S_1(h) x ds \right\| \leq M_1 e^{|w_1|h} M_2 e^{|w_2|h} \hat{C}(\|A_1^2 x\| + \|x\|) \frac{h^2}{2}, \tag{4.84}$$

For the term (4.76), using (Lemma 4.1) to compare A_1 and A_2, we have

$$\left\| hA_2 \int_0^h S_1(s)A_1 x ds \right\| \leq h\hat{\mathcal{C}} \left(\left\| A_1 \int_0^h S_1(s)A_1 x ds \right\| + \left\| \int_0^h S_1(s)A_1 x ds \right\| \right) \tag{4.85}$$

Using (4.61) twice and the fact that all semigroups commute with their generator, we get

$$A_1 \int_0^h S_1(s) A_1 x ds = S_1(h) A_1 x - A_1 x = \int_0^h S_1(s) A_1^2 x ds, \tag{4.86}$$

Hence we get the estimate,

$$\begin{aligned} \left\| h A_2 \int_0^h S_1(s) A_1 x ds \right\| &\leq h\hat{C} \left(\left\| \int_0^h S_1(s) A_1^2 x ds \right\| + \left\| \int_0^h S_1(s) A_1 x ds \right\| \right) & (4.87) \\ &\leq h^2 \hat{C} M_1 e^{|w_1| h} (\|A_1^2 x\| + \|x\|) & (4.88) \end{aligned}$$

Hence, adding the four estimates (4.80),(4.81), (4.84) and (4.87), we get the following,

$$\|S_2(h)S_1(h)x - S(h)x\| \leq h^2 C(T)(\|A_1^2 x\| + \|x\| + \|A^2 x\| + \|x\|) \tag{4.89}$$

From Lemma 4.1 we know that we can bound $\|A_1^2 x\|$ in terms of $\|A^2 x\| + \|x\|$ and similarly $\|A_1 x\|$ in terms of $\|A^2 x\| + \|x\|$. □

To prove the first-order consistency of the Lie-Trotter splitting, we need a uniform bound, proportional to h^2 on

$$\|S_2(h)S_1(h)u(t) - S(h)u(t)\| \tag{4.90}$$

as t runs from 0 to $T - h$, where $u(t) = S(t)u_0$ is the exact solution of the original problem (4.44)-(4.45).

Proposition (4.1), (4.64) and Lemma (4.2) imply the following

Theorem 4.5 *Let the conditions of Proposition (4.1) be satisfied. Then for any* $u_0 \in D$ *we have a uniform bound*

$$\|S_2(h)S_1(h)u(t) - S(h)u(t)\| \leq h^2 C(T) \tag{4.91}$$

where $C(T)$ is a constant independent of h.

4.2.3. Consistency of the Symmetrically Weighted Splitting

Our aim is to show the second order consistency of the Symmetrically Weighted Splitting for C_0-semigroups. By using (4.59) for $n = 3$, for $x \in D(A)$ we then have,

$$S_2(h)S_1(h)x = S_1(h)x + hA_2S_1(h)x + \frac{h^2}{2}A_2^2S_1(h)x \quad (4.92)$$

$$+\frac{1}{2}\int_0^h (h-s)^2 S_2(s)A_2^3S_1(h)xds \quad (4.93)$$

and similarly,

$$S_1(h)S_2(h)x = S_2(h)x + hA_1S_2(h)x + \frac{h^2}{2}A_1^2S_2(h)x \quad (4.94)$$

$$+\frac{1}{2}\int_0^h (h-s)^2 S_1(s)A_1^3S_2(h)xds \quad (4.95)$$

Applying (4.60), (4.61) and (4.62) for the semigroups $\{S_1(t)\}_{t\geq 0}$ and $\{S_2(t)\}_{t\geq 0}$ and substituting the corresponding expressions into the first, second and third terms of the right-hand side of (4.92), we get

$$\frac{1}{2}(S_2(h)S_1(h) + S_1(h)S_2(h)x) = \quad (4.96)$$

$$x + h(A_1 + A_2)x + \frac{h^2}{2}(A_1 + A_2)^2x \quad (4.97)$$

$$+\frac{1}{4}\int_0^h (h-s)^2 S_1(s)A_1^3xds \quad (4.98)$$

$$+\frac{1}{4}\int_0^h (h-s)^2 S_2(s)A_2^3xds \quad (4.99)$$

$$+\frac{1}{2}hA_2\int_0^h (h-s)S_2(s)A_1^2xds + \frac{1}{2}hA_1\int_0^h (h-s)S_2(s)A_2^2xds \quad (4.100)$$

$$+\frac{1}{4}h^2A_2^2\int_0^h S_1(s)A_1xds+\frac{1}{4}h^2A_1^2\int_0^h S_2(s)A_2xds \tag{4.101}$$

$$+\frac{1}{4}\int_0^h (h-s)^2S_2(s)A_2^3S_1(h)xds+\frac{1}{4}\int_0^h (h-s)^2S_1(s)A_1^3S_2(h)xds \tag{4.102}$$

On the other hand, we have

$$S(h)x=x+hAx+\frac{h^2}{2}A^2x+\frac{1}{2}\int_0^h (h-s)^2S(s)A^3xds \tag{4.103}$$

so the difference is

$$\frac{1}{2}(S_2(h)S_1(h)+S_1(h)S_2(h)x)-S(h)x= \tag{4.104}$$

$$+\frac{1}{4}\int_0^h (h-s)^2S_1(s)A_1^3xds+\frac{1}{4}\int_0^h (h-s)^2S_2(s)A_2^3x \tag{4.105}$$

$$+\frac{1}{2}hA_2\int_0^h (h-s)S_1(s)A_1^2xds+\frac{1}{2}hA_1\int_0^h (h-s)S_2(s)A_2^2xds \tag{4.106}$$

$$+\frac{1}{4}h^2A_2^2\int_0^h S_1(s)A_1xds+\frac{1}{4}h^2A_1^2\int_0^h S_2(s)A_2xds \tag{4.107}$$

$$+\frac{1}{4}\int_0^h (h-s)^2S_2(s)A_2^3S_1(h)xds+\frac{1}{4}\int_0^h (h-s)^2S_1(s)A_1^3S_2(h)xds \tag{4.108}$$

$$-\frac{1}{2}\int_0^h (h-s)^2S(s)A^3xds \tag{4.109}$$

Proposition 4.2 *Let A, A_1 and A_2 be infinitesimal generators of the C_0-semigroups $\{S(t)\}_{t\geq 0}$, $\{S_1(t)\}_{t\geq 0}$ and $\{S_2(t)\}_{t\geq 0}$, respectively,. Assume that (4.53) and (4.54) are satisfied, and let $T>0$. Then for all $x\in D$ the relation*

$$\left\|\frac{1}{2}(S_2(h)S_1(h)+S_1(h)S_2(h)x)-S(h)x\right\|\leq \tag{4.110}$$

$$h^3C(T)(\|A^3x\|+\|A^2x\|+\|Ax\|+\|x\|) \tag{4.111}$$

holds $h \in [0, T]$, where $C(T)$ is a constant of independent of h.

Proof We estimate the terms on the right-hand side of (4.104)-(4.109). For the first term in (4.106) by using (Lemma 4.1) we can write

$$\left\| \frac{1}{2} h A_2 \int_0^h (h-s) S_1(s) A_1^2 x ds \right\| \leq \frac{\hat{C}}{2} h \left\| A_1 \int_0^h (h-s) S_1(s) A_1^2 x ds \right\| \quad (4.112)$$

$$+ \frac{\hat{C}}{2} h \left\| \int_0^h (h-s) S_1(s) A_1^2 x ds \right\| \quad (4.113)$$

Using (4.61) twice and the fact that all semigroups commute with their generator, for the term (4.112) we obtain the estimate

$$\frac{\hat{C}}{2} h \left\| A_1 \int_0^h (h-s) S_1(s) A_1^2 x ds \right\| \leq M_1 e^{|w_1| h} \| A_1^3 x \| \frac{h^3}{4} \hat{C}. \quad (4.114)$$

Term (4.113) can be estimated by

$$\frac{\hat{C}}{2} h \left\| \int_0^h (h-s) S_1(s) A_1^2 x ds \right\| \leq M_1 e^{|w_1| h} \| A_1^2 x \| \frac{h^3}{4} \hat{C}. \quad (4.115)$$

So,

$$\left\| \frac{1}{2} h A_2 \int_0^h (h-s) S_1(s) A_1^2 x ds \right\| \leq M_1 e^{|w_1| h} (\| A_1^3 x \| + \| A_1^2 x \|) \frac{h^3}{4} \hat{C}. \quad (4.116)$$

Similarly, for the second term in (4.106) the following relation is valid,

$$\left\| \frac{1}{2} h A_1 \int_0^h (h-s) S_2(s) A_2^2 x ds \right\| \leq M_2 e^{|w_2| h} (\| A_2^3 x \| + \| A_2^2 x \|) \frac{h^3}{4} \hat{C}. \quad (4.117)$$

For the estimate of he first term of (4.107) on the base of (Lemma 4.1) we can write

$$\left\|\frac{1}{4}h^2A_2^2\int_0^h S_1(s)A_1xds\right\| \leq \frac{\hat{C}}{4}h^2\left\|A_1^2\int_0^h (h-s)S_1(s)A_1xds\right\| \quad (4.118)$$

$$+\frac{\hat{C}}{4}h^2\left\|\int_0^h (h-s)S_1(s)A_1xds\right\| \quad (4.119)$$

where for terms (4.118) we have

$$\frac{\hat{C}}{4}h^2\left\|A_1^2\int_0^h (h-s)S_1(s)A_1xds\right\| = \frac{\hat{C}}{4}h^2\left\|\int_0^h (h-s)S_1(s)A_1^3xds\right\| \quad (4.120)$$

$$\leq \frac{\hat{C}}{4}h^3M_1e^{|w_1|h}\|A_1^3x\| \quad (4.121)$$

and for the term (4.119),

$$\frac{\hat{C}}{4}h^2\left\|\int_0^h (h-s)S_1(s)A_1xds\right\| \leq \frac{\hat{C}}{4}h^3M_1e^{|w_1|h}\|A_1x\| \quad (4.122)$$

Consequently,

$$\left\|\frac{1}{4}h^2A_2^2\int_0^h S_1(s)A_1xds\right\| \leq M_1e^{|w_1|h}\hat{C}(\|A_1^3x\|+\|A_1x\|)\frac{h^3}{4}. \quad (4.123)$$

In a similar way, the second term of (4.107) is estimated by

$$\left\|\frac{1}{4}h^2A_1^2\int_0^h S_2(s)A_2xds\right\| \leq M_2e^{|w_2|h}\hat{C}(\|A_2^3x\|+\|A_2x\|)\frac{h^3}{4}. \quad (4.124)$$

For the first term of (4.108) we can write

$$\left\| \frac{1}{4} \int_0^h (h-s)^2 S_2(s) A_2^3 S_1(h) x ds \right\| \leq M_2 e^{|w_2|h} \|A_2^3 S_1(h) x\| \frac{h^3}{12} \quad (4.125)$$

$$\leq M_2 e^{|w_2|h} \hat{C} (\|A_1^3 S_1(h) x\| + \|S_1(h) x\|) \frac{h^3}{12} \quad (4.126)$$

$$\leq M_1 e^{|w_1|h} M_2 e^{|w_2|h} \hat{C} (\|A_1^3 x\| + \|x\|) \frac{h^3}{12} \quad (4.127)$$

Finally, in a similar manner, the second term of (4.108) is estimated by

$$\left\| \frac{1}{4} \int_0^h (h-s)^2 S_1(s) A_1^3 S_2(h) x ds \right\| \leq \quad (4.128)$$

$$M_1 e^{|w_1|h} M_2 e^{|w_2|h} \hat{C} (\|A_2^3 x\| + \|A_2 x\|) \frac{h^3}{12}. \quad (4.129)$$

□

To prove the second-order consistency of the Symmetrically weighted splitting, we need a uniform bound, proportional to h^3 on

$$\|\frac{1}{2}(S_2(h)S_1(h)u(t) + S_1(h)S_2(h)u(t)) - S(h)u(t)\| \quad (4.130)$$

as t runs from 0 to $T-h$, where $u(t) = S(t)u_0$ is the exact solution of the original problem (4.44)-(4.45).

Proposition (4.2), (4.64) and Lemma (4.2) imply the following

Theorem 4.6 *Let the conditions of Proposition (4.2) be satisfied. Then for any* $u_0 \in D$ *we have a uniform bound*

$$\left\| \frac{1}{2}(S_2(h)S_1(h)u(t) + S_1(h)S_2(h)u(t)) - S(h)u(t) \right\| \leq h^3 C(T) \quad (4.131)$$

where $C(T)$ *is a constant independent of h.*

4.2.4. Consistency of the Strang Splitting

Let us introduce the notation $y = S_2(h)S_1(h/2)$, and let $x \in D$ according to (4.54). Then we can write

$$S_1(h/2)S_2(h)S_1(h/2) = S_1(h/2)y \tag{4.132}$$

and by (4.59) we have

$$S_1(h/2)y = y + \frac{h}{2}A_1 y + \frac{h^2}{8}A_1^2 y + \frac{1}{2}\int_0^{h/2}(\frac{h}{2} - s)^2 S_1(s)A_1^3 y ds \tag{4.133}$$

Substituting

$$\begin{aligned} y &= S_1(h/2)x + hA_2S_1(h/2)x + \frac{h^2}{2}A_2^2S_1(h/2)x && (4.134)\\ &+\frac{1}{2}\int_0^h (h-s)^2 S_2(s)A_2^3S_1(h/2)xds && (4.135)\\ y &= S_1(h/2)x + hA_2S_1(h/2)x + \int_0^h (h-s)S_2(s)A_2^2S_1(h/2)xds && (4.136)\\ y &= S_1(h/2)x + \int_0^h S_2(s)A_2S_1(h/2)xds && (4.137)\end{aligned}$$

and

$$y = S_2(h)S_1(h/2)x \tag{4.138}$$

successively the terms of the right-hand side of (4.133), and the expressions

$$S_1(h/2)x = x + \frac{h}{2}A_1 x + \frac{h^2}{8}A_1^2 x + \frac{1}{2}\int_0^{h/2}(\frac{h}{2} - s)^2 S_1(s)A_1^3 x ds \tag{4.139}$$

$$S_1(h/2)x = x + \frac{h}{2}A_1x + \int_0^{h/2}(\frac{h}{2} - s)S_1(s)A_1^2xds \quad (4.140)$$

$$S_1(h/2)x = x + \int_0^{h/2} S_1(s)A_1xds \quad (4.141)$$

Taking into account (4.103), we obtain that

$$S_1(h/2)S_2(h)S_1(h/2)x - S(h)x = \quad (4.142)$$

$$+\frac{1}{2}\int_0^{h/2}(\frac{h}{2} - s)^2S_1(s)A_1^3xds + hA_2\int_0^{h/2}(\frac{h}{2} - s)S_1(s)A_1^2xds \quad (4.143)$$

$$+\frac{h^2}{2}A_2^2\int_0^{h/2} S_1(s)A_1xds + \frac{1}{2}\int_0^{h}(h - s)^2S_2(s)A_2^3S_1(h/2)xds \quad (4.144)$$

$$+\frac{h}{2}A_1\int_0^{h/2}(\frac{h}{2} - s)S_1(s)A_1^2xds + \frac{h^2}{2}A_1A_2\int_0^{h/2} S_1(s)A_1xds \quad (4.145)$$

$$+\frac{h}{2}A_1\int_0^{h}(h - s)S_2(s)A_2^2S_1(h/2)xds + \frac{h^2}{8}A_1^2\int_0^{h/2} S_1(s)A_1xds \quad (4.146)$$

$$+\frac{h^2}{8}A_1^2\int_0^{h} S_2(s)A_2S_1(h/2)xds \quad (4.147)$$

$$+\frac{1}{2}\int_0^{h/2}(\frac{h}{2} - s)^2S_1(s)A_1^3S_2(h)S_1(h/2)xds \quad (4.148)$$

$$-\frac{1}{2}\int_0^{h}(h - s)^2S(s)A^3xds \quad (4.149)$$

Proposition 4.3 *Let A, A_1 and A_2 be infinitesimal generators of the C_0-semigroups $\{S(t)\}_{t\geq 0}$, $\{S_1(t)\}_{t\geq 0}$ and $\{S_2(t)\}_{t\geq 0}$, respectively,. Assume that (4.53) and (4.54) are satisfied, and let $T > 0$. Then for all $x \in D$ the relation*

$$\|S_1(h/2)S_2(h)S_1(h/2)x - S(h)x\| \leq \quad (4.150)$$

$$h^3C(T)(\|A^3x\| + \|A^2x\| + \|Ax\| + \|x\|) \quad (4.151)$$

holds $h \in [0, T]$, *where* $C(T)$ *is a constant of independent of h.*

Proof We estimate the terms on the right-hand side of (4.142)-(4.149) one by one. The first term of (4.143) can be directly estimated as

$$\frac{1}{2}\left\|\int_0^{h/2}(\frac{h}{2}-s)^2 S_1(s)A_1^3 x ds\right\| \leq M_1 e^{|w_1|h/2}\|A_1^3 x\|\frac{h^3}{48} \quad (4.152)$$

For the second term of (4.143) by the use of (Lemma 4.1) we can write

$$\left\|hA_2\int_0^{h/2}(\frac{h}{2}-s)S_1(s)A_1^2 x ds\right\| \leq \hat{C}h\left\|A_1\int_0^{h/2}(\frac{h}{2}-s)S_1(s)A_1^2 x ds\right\| \quad (4.153)$$

$$+\hat{C}h\left\|\int_0^{h/2}(\frac{h}{2}-s)S_1(s)A_1^2 x ds\right\| \quad (4.154)$$

Here by using (4.61) twice, for the first integral can be written as

$$A_1\int_0^{h/2}(\frac{h}{2}-s)S_1(s)A_1^2 x ds = \int_0^{h/2}(\frac{h}{2}-s)S_1(s)A_1^3 x ds \quad (4.155)$$

and so the term (4.153) can be estimated by

$$M_1 e^{|w_1|h/2}\|A_1^3 x\|\frac{h^3}{8}\hat{C} \quad (4.156)$$

For the term (4.154) the following estimates holds

$$M_1 e^{|w_1|h/2}\|A_1^2 x\|\frac{h^3}{8}\hat{C} \quad (4.157)$$

The first term of (4.144) we have

$$\left\| \frac{h^2}{2} A_2^2 \int\limits_0^{h/2} S_1(s) A_1 x ds \right\| \leq M_1 e^{|w_1| h/2} (\|A_1^3 x\| + \|A_1 x\|) \frac{h^3}{4} \tag{4.158}$$

The second term of (4.144) can be estimated as

$$\frac{1}{2} \left\| \int\limits_0^{h} (h-s)^2 S_2(s) A_2^3 S_1(h/2) x ds \right\| \leq \frac{1}{2} M_2 e^{|w_2| h} \|A_2^3 x S_1(h/2)\| \frac{h^3}{3} \tag{4.159}$$

From the (Lemma 4.1) we get the right-hand side of (4.159)

$$M_1 e^{|w_1| h/2} M_2 e^{|w_2| h} \hat{C} (\|A_1^3 x\| + \|x\|) \frac{h^3}{6} \tag{4.160}$$

For the first term of (4.145) we can write

$$\frac{h}{2} \left\| A_1 \int\limits_0^{h/2} (\frac{h}{2} - s) S_1(s) A_1^2 x ds \right\| \leq M_1 e^{|w_1| h/2} \|A_1^3 x\| \frac{h^3}{16} \tag{4.161}$$

For the second term one has

$$\left\| \frac{h^2}{2} A_1 A_2 \int\limits_0^{h/2} S_1(s) A_1 x ds \right\| \leq \hat{C} \frac{h^2}{2} \|A_2^2 \int\limits_0^{h/2} S_1(s) A_1 x ds\| \tag{4.162}$$

$$+ \hat{C} \frac{h^2}{2} \|A_2 \int\limits_0^{h/2} S_1(s) A_1 x ds\| \tag{4.163}$$

which, by Lemma (4.1), is less than or equal to

$$M_1 e^{|w_1| h/2} \hat{C}^2 (\|A_1^3 x\| + \|A_1^2 x\| + 2\|A_1 x\|) \frac{h^3}{4} \tag{4.164}$$

Using again Lemma (4.1), the first term of (4.146) can be estimated as

$$\frac{h}{2}\left\|A_1\int_0^h (h-s)S_2(s)A_2^2S_1(h/2)xds\right\| \tag{4.165}$$

$$\leq \frac{h}{2}\hat{C}(\|A_2\int_0^h (h-s)S_2(s)A_2^2S_1(h/2)xds\|) \tag{4.166}$$

$$+\|\int_0^h (h-s)S_2(s)A_2^2S_1(h/2)xds\| \tag{4.167}$$

$$\leq M_2e^{|w_2|h}M_1e^{|w_1|h/2}\hat{C}^2(\|A_1^3x\|+\|A_1^2x\|+2\|A_1x\|)\frac{h^3}{4} \tag{4.168}$$

For the second term of (4.146) we have

$$\frac{h^2}{8}\left\|A_1^2\int_0^{h/2} S_1(s)A_1xds\right\| \leq M_1e^{|w_1|h/2}\|A_1^3x\|\frac{h^3}{16} \tag{4.169}$$

We estimate the (4.147) as

$$\begin{aligned}
&\frac{h^2}{8}\left\|A_1^2\int_0^h S_2(s)A_2S_1(h/2)xds\right\| \\
&\leq \frac{h^2}{8}\hat{C}\left\|A_2^2\int_0^h S_2(s)A_2S_1(h/2)xds\right\| + \frac{h^2}{8}\hat{C}\left\|\int_0^h S_2(s)A_2S_1(h/2)xds\right\| \\
&\leq \frac{h^3}{8}\hat{C}^2M_2e^{|w_2|h}\|A_2^3S_1(h/2)x\| + \frac{h^3}{8}\hat{C}^2M_2e^{|w_2|h}\|A_2S_1(h/2)x\| \\
&\leq M_1e^{|w_1|h/2}M_2e^{|w_2|h}\hat{C}^2(\|A_1^3x\|+\|A_1x\|+2\|x\|)\frac{h^3}{8}
\end{aligned} \tag{4.170}$$

and the (4.148)

$$\frac{1}{2}\left\|\int_0^{h/2}(\frac{h}{2}-s)^2S_1(s)A_1^3S_2(h)S_1(h/2)xds\right\| \leq \tag{4.171}$$

$$\leq \frac{h^3}{48}M_1e^{|w_1|h/2}\hat{C}(\|A_2^3S_2(h)S_1(h/2)x\|+\|S_2(h)S_1(h/2)x\|) \tag{4.172}$$

Here

$$\|A_2^3 S_2(h) S_1(h/2)x\| \leq M_2 e^{|w_2|h} \|A_2^3 S_1(h/2)x\| \tag{4.173}$$

$$\leq M_2 e^{|w_2|h} \hat{C}(\|\|A_1^3 S_1(h/2)x\| + \|S_1(h/2)x\|). \tag{4.174}$$

Therefore

$$\frac{1}{2}\left\|\int_0^{h/2} (\frac{h}{2}-s)^2 S_1(s) A_1^3 S_2(h) S_1(h/2) x ds\right\| \leq \tag{4.175}$$

$$M_1 e^{|w_1|h/2} M_2 e^{|w_2|h} M_1 e^{|w_1|h/2} (\hat{C}^2(\|A_1^3 x\| + \|x\|) + \hat{C}\|x\|)\frac{h^3}{48} \tag{4.176}$$

Finally, for the term (4.149) we have

$$\frac{1}{2}\left\|\int_0^{h} (h-s)^2 S(s) A^3 x ds\right\| \leq \frac{1}{2} M e^{|w|h} \|A^3 x\| \frac{h^3}{3}. \tag{4.177}$$

□

Proposition (4.3), (4.64) and Lemma 4.2 imply the following

Theorem 4.7 *Let the conditions of Proposition (4.3) be satisfied. Then for any* $u_0 \in D$ *we have a uniform bound*

$$\|S_1(h/2) S_2(h) S_1(h/2) x - S(h)x\| \leq h^3 C(T) \tag{4.178}$$

where $C(T)$ *is a constant independent of* h*.*

CHAPTER 5

STABILITY ANALYSIS FOR OPERATOR SPLITTING METHODS

In this chapter, we will discuss the stability analysis of the operator splitting methods for ODE systems and PDE problems, such that nonlinear KdV equation. For PDE sense we will use the Von-Neumann stability analysis. General approach to Von-Neumann stability analysis for Lie-Trotter and Strang splitting will be discussed.

5.1. Stability for Linear ODE Systems

In this section, we take a look at properties of linear systems of ODEs and in particular at influence of perturbations at such systems.

Consider the initial value problem,

$$\frac{\partial U(t)}{\partial t} = AU(t), \text{ with } t \in [0, T], \; U(0) = U_0, \tag{5.1}$$

with given matrix $A \in \mathbb{R}^{m \times m}$. The solution of the equation (5.1) can be written as,

$$U(t) = e^{tA} U_0. \tag{5.2}$$

Consider also a perturbed problem,

$$\frac{\partial \hat{U}(t)}{\partial t} = A\hat{U}(t) + \delta(t), \text{ with } t \in [0, T], \; \hat{U}(0) = \hat{U}_0, \tag{5.3}$$

Then for $\varepsilon(t) = \hat{U}(t) - U(t)$ we find by the variation of constant formula that,

$$\varepsilon(t) = e^{tA}\varepsilon(0) + \int_0^t e^{(t-s)A}\delta(s)ds, \tag{5.4}$$

which leads to the norm estimate

$$\|\varepsilon(t)\| \leq \|e^{tA}\|\|\varepsilon(0)\| \ + \int_0^t \|e^{(t-s)A}\|ds \ \max_{0\leq s\leq t} \|\delta(s)\|. \tag{5.5}$$

Consequently, if we have the following stability inequality

$$\|e^{tA}\| \leq Ke^{tw} \quad \text{for all } \ t \geq 0, \tag{5.6}$$

with constants $K > 0$ and $w \in \mathbb{R}$, then we obtain

$$\|\varepsilon(t)\| \leq Ke^{tw}\|\varepsilon(0)\| + \frac{K}{t}(e^{tw} - 1) \max_{0\leq s\leq t} \|\delta(s)\|, \tag{5.7}$$

with convention $(e^{tw} - 1)/w = t$ in case $w = 0$. This inequality shows that the overall error $\|\varepsilon(t)\|$ can be bounded in terms of the initial error $\|\varepsilon(0)\|$ and perturbations $\|\delta(s)\|$, $0 \leq s \leq t$.

In general, the term stability will be used to indicate that small perturbations give a small overall effect. We now take a closer look at bounds for $\|e^{tA}\|$. Suppose that A is diagonalizable, $A = P\Lambda P^{-1}$, where $\Lambda = \text{diag}(\lambda_k)$ and that the vector norm is absolute. Then it follows that,

$$\|e^{tA}\| \leq \|P\|\|\Lambda\|\|P^{-1}\| = cond(P) \max_{1\leq k\leq m} |e^{t\lambda_k}|. \tag{5.8}$$

Consequently, if we know that $cond(P) = \|P\|\|P^{-1}\| \ \leq K$ and $Re\lambda_k \leq w$, then (5.6) follows with

$$w = \max_{1\leq k\leq m} |e^{t\lambda_k}|. \tag{5.9}$$

In particular, if A is normal matrix, then the matrix of eigenvectors P is unitary. Since $e^{tA} = Pe^{t\Lambda}P^{-1}$ the matrix e^{tA} is also normal. Thus with the normal matrices A we have

$$\|e^{tA}\|_2 = \max_{1\leq k\leq m} |e^{t\lambda_k}|. \tag{5.10}$$

Assume for A, two-term splitting in (5.1),

$$A = A_1 + A_2 \tag{5.11}$$

The solution of (5.1) is given by

$$U(t_{n+1}) = e^{tA}U(t_n) \tag{5.12}$$

where $t = t_{n+1} - t_n$ on each subintervals $[t^n, t^{n+1}]$, where $n = 0, 1, ..., N-1$. If we wish to use only A_1 and A_2 separately, instead of the full A, then (5.12) can be approximated by

$$U_{n+1} = e^{tA_2}e^{tA_1}U_n \tag{5.13}$$

with U_n approximating $U(t_n)$. With regard to stability, if we have $\|e^{tA_k}\| \leq 1$, $k = 1, 2$, then it follows trivially that $\|U_{n+1}\| \leq \|U_n\|$ for the splitting (5.13). General stability results under the weaker assumption that $\|e^{tA_k}\| \leq K$ for $0 \leq t \leq T$ with a constant $K \geq 1$ seem unknown. However, in practice the splitting appears to be stable provided the sub-steps themselves are stable.

In general, if the matrix A is not normal, an estimate of cond(U) in some suitable norm maybe difficult to obtain. For this reason we will look a more general concept to obtain bounds for $\|e^{tA}\|$. A useful concept for stability results with non-normal matrices is the logarithmic norm of a matrix A in $\mathbb{R}^{m\times m}$, defined as

$$\mu(A) = \lim_{t\downarrow 0} \frac{\|I + tA\|}{t}. \tag{5.14}$$

In terms of logarithmic matrix norms, $\|e^{tA_k}\| \leq 1$ means that $\mu(A_k) \leq 0$. This implies

$\mu(A_1 + A_2) \leq 0$ and therefore $\|e^{t(A_1+A_2)}\| \leq 1$, so the system will be stable.

5.2. Stability Analysis for PDE

In order to determine the Courant-Friedrichs-Levy condition for the stability of an explicit solution of a PDE the Von Neumann stability analysis is used. A very versatile tool for analysing stability is the Fourier method developed by Von Neumann. Here initial values at mesh points are expressed in terms of a finite Fourier series, and we consider the growth of individual Fourier components. We do not need to find eigenvalues, or matrix norms.

A unique representation of the function $U(x)$ can be expressed as,

$$U(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{U}(\xi) e^{i\xi x} d\xi \tag{5.15}$$

Consider a trial solution at x,

$$U(x,t) = U(t)e^{ikx} \tag{5.16}$$

We can write the U_j^n and U_j^{n+1} as follows,

$$U_j^n = U(x_j, t_n) = \hat{U}^n e^{ikjh} \tag{5.17}$$

$$U_j^{n+1} = U(x_j, t_{n+1}) = \hat{U}^{n+1} e^{ikjh} \tag{5.18}$$

The amplification factor is so called because its magnitude is the amount of the amplitude of each frequency in the solution given by,

$$\rho(\xi) = \frac{\hat{U}^{n+1}}{\hat{U}^n} \tag{5.19}$$

Where $\xi =$ kjh. If $|\xi| \leq 1$ then the solution dampened. If $|\xi| > 1$ the solution grows in amplitude and becomes unstable.

We illustrate the method by considering the particular example. Through the use of Fourier transform the determination of the stability of a scheme is reduced to relatively simple algebraic consideration.

We consider the following problem parabolic problem:

$$u_t = Du_{xx}, \tag{5.20}$$

Let $x_i = i\Delta x$ and $t_n = n\Delta t, \quad i = 1, ..., M-1 \;\; n = 0, ..., N$ Respectively $\Delta x = \frac{1}{M}$ $\Delta t = \frac{1}{N}$ are the regular spatial end time step sizes. The discrete representation of (5.20) over each time interval $[t_n, t_n + \Delta t]$ is as follows,

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = \frac{D}{\Delta x^2}(U_{i+1}^{n+1} - 2U_i^{n+1} + U_{i-1}^{n+1}) \tag{5.21}$$

Let say $\frac{D\Delta t}{\Delta x^2} = r$. Rearranging the terms (5.21) according to the time level, then

$$-rU_{i+1}^{n+1} + (1+2r)U_i^{n+1} - rU_{i-1}^{n+1} = U_i^n \tag{5.22}$$

The discrete Fourier transform of (5.22) is given by,

$$(-re^{i\xi} + (1+2r) - re^{-i\xi})\hat{U}^{n+1} = \hat{U}^n \tag{5.23}$$

After simplification (5.23) reduce to

$$(1 + 4r\sin^2 \xi/2)\hat{U}^{n+1} = \hat{U}^n \tag{5.24}$$

and amplification factor corresponding to (5.24) is given by,

$$\rho(\xi) = \frac{1}{1 + 4r\sin^2 \xi/2} \tag{5.25}$$

The stability of the solution obtained by the diffusion operator satisfies that,

$$|\rho(\xi)| < 1 \tag{5.26}$$

for any value of $r > 0$ for any positive scalar coefficient of the diffusion operator.

5.3. Stability Analysis of the Non-linear KdV Equation

In this section, we first give the numerical algorithms then present the Von Neumann stability analysis for the nonlinear KdV equation by appling Lie-Trotter and Strang splitting methods and give the stability conditions related to these methods.

In 1895, Korteweg and de Vries formulated the equation

$$U_t - 6UU_x + U_{xxx} = 0 \tag{5.27}$$

which models Russell's observation.The term UU_x describes the sharpening of the wave and U_{xxx} the dispersion. Let $x_i = i\Delta x$ and $t_n = n\Delta t, \quad i = 1, ..., M-1 \;\; n = 0, ..., N$ Respectively $\Delta x = \frac{1}{M}$ $\Delta t = \frac{1}{N}$ are the regular spatial end time step sizes. The first step towards solving (5.27) is to consider the fractional splitting method, which can be expressed as follows:

$$u_t = -u_{xxx}\,, \quad t \in [t_n, t_n + \Delta t]\,, \tag{5.28}$$

$$v_t = 6uv_x, \quad t \in [t_n, t_n + \Delta t]\,,\; v(t_n) = u(t_n + \Delta t)\,. \tag{5.29}$$

We substitute the solution of the equation (6.36) for u in (6.37),

We imply the semi-discretisation for (5.27) using the central difference approximation. The finite difference approximation of the operators (5.27) are given by,

$$\begin{aligned} (6u\frac{\partial u}{\partial x} - \frac{\partial^3 u}{\partial x^3})_{(x_i,t)} &= 6u\frac{1}{2\Delta x}(u_{i+1}(t) - u_{i-1}(t)) \\ &- \frac{1}{2\Delta x^3}(u_{i+2}(t) - 2u_{i+1}(t) + 2u_{i-1}(t) - u_{i-2}(t)) \end{aligned} \tag{5.30}$$

We will take u as a constant in here, for $i = 1, ..., N$ We obtain the following system of the first order differential equation,

$$u_t = Au \tag{5.31}$$

$$v_t = Bv \tag{5.32}$$

where A and B are global matrices of coefficients resulting from he discretisation of $-uxxx$ and v_x

$$A = -\frac{1}{2\Delta x^3}[1 \quad -2 \ \ 2 \quad -1] \tag{5.33}$$

$$B = 6c\frac{1}{2\Delta x}[-1 \ \ 0 \ \ 1] \tag{5.34}$$

We will obtain the following system of first order differential equation given by,

$$\frac{\partial u^*}{\partial t} = (A + B)u^* \tag{5.35}$$

The exact solution of (5.35) satisfies the matrix exponential function of the matrices A and B given by,

$$u^*(t + \Delta t) = e^{\Delta t(A+B)}u^*(t) \tag{5.36}$$

where Δt is the time step for the simulation of of the solution through $[0, T]$

5.3.1. Algorithm 1 (First Order Splitting Method)

Over the time interval $[t_n, t_n + \Delta t]$

- Step1:

$$u(t_n + \Delta t) = e^{\Delta t A}u(t_n) \ \text{ with } \ u(t_n) = u^*(t_n) \tag{5.37}$$

- Step2:

$$v(t_n + \Delta t) = e^{\Delta t B} v(t_n) \ \text{ with } \ v(t_n) = u(t_n + \Delta t) \tag{5.38}$$

- Step3:

$$u^*(t_n + \Delta t) = v(t_n + \Delta t) \tag{5.39}$$

- Step4: If $T < (n+1)\Delta t$ go to Step1, otherwise stop.

The recurrence solution given by (5.37) and (5.38) will be estimated using the Pade' approximation for $e^{\Delta t A}$ and $e^{\Delta t B}$, respectively (Daoud, 2007)

$$\begin{aligned} e^{\Delta t A} &= (I - \Delta t A)^{-1} + O(\Delta t^2) \ , \\ e^{\Delta t B} &= (I - \Delta t B)^{-1} + O(\Delta t^2), \end{aligned} \tag{5.40}$$

which is locally second order approximation in time $O(\Delta t^2)$.Therefore,

$$e^{\Delta t(A+B)} \simeq e^{\Delta t A} e^{\Delta t B} \simeq (I - \Delta t A)^{-1} (I - \Delta t B)^{-1} O(\Delta t^2) \simeq (I - \Delta t A)^{-1} \tag{5.41}$$

We could easily observe that

$$u(t_n + \Delta t) = e^{\Delta t A} e^{\Delta t B} u(t_n) \simeq e^{\Delta t (A+B)} \tag{5.42}$$

The discrete presentation of (5.37) and (5.38) using (5.57) over each time interval $[t_n, t_n + \Delta t]$ are as follows

$$\begin{aligned} \frac{u_i^{n+1} - u_i^n}{\Delta t} &= -\frac{1}{2\Delta x^3}(u_{i+2}^{n+1} - 2u_{i+1}^{n+1} + 2u_{i-1}^{n+1} - u_{i-2}^{n+1}) \ , \\ \frac{v_i^{n+1} - v_i^n}{\Delta t} &= \frac{1}{2\Delta x}(v_{i+1}^{n+1} - v_{i-1}^{n+1}) \end{aligned} \tag{5.43}$$

Let $\frac{6c\Delta t}{2\Delta x} = R$ and $\frac{\Delta t}{2\Delta x^3} = r$ Rearranging the terms of (5.43) according to the time level, then

$$\begin{aligned} ru_{i+2}^{n+1} - 2ru_{i+1}^{n+1} + 2ru_{i-1}^{n+1} - ru_{i-2}^{n+1} + u_i^{n+1} &= u_i^n , \\ -Rv_{i+1}^{n+1} + v_i^{n+1} + Rv_{i-1}^{n+1} &= v_i^n \end{aligned} \tag{5.44}$$

Next, we will investigate the stability analysis of Lie-Trotter splitting.

5.3.2. Stability Analysis of the Lie-Trotter Splitting

Theorem 5.1 *For any Δt and Δx the First Order Splitting Method (Lie-Trotter Splitting) is stable in ℓ_2 norm.*

Proof For stability of the ℓ_2 norm we will consider the Von-Neumann stability analysis and using the discrete Fourier transform. The discrete Fourier transform is given by

$$\begin{aligned} \hat{u}^n e^{i\xi} &= r\hat{u}^{n+1}e^{(i+2)\xi} - 2r\hat{u}^{n+1}e^{(i+1)\xi} + 2r\hat{u}^{n+1}e^{(i-1)\xi} \\ &\quad + r\hat{u}^{(d)n+1}e^{(i-2)\xi} + \hat{u}^{(d)n+1}e^{i\xi} \\ \hat{v}^n e^{i\xi} &= -R\hat{v}^{n+1}e^{(i+1)\xi} + \hat{v}^{n+1}e^{i\xi} + R\hat{v}^{n+1}e^{(i-1)\xi} \end{aligned} \tag{5.45}$$

rearanging the terms in (5.45) we get,

$$\begin{aligned} \hat{u}^n &= (re^{2i\xi} - 2re^{i\xi} + 2re^{-i\xi} - re^{-2i\xi} + 1)\hat{u}^{n+1} \\ \hat{v}^n &= (-Re^{i\xi} + 1 + Re^{-i\xi})\hat{v}^{n+1} \end{aligned} \tag{5.46}$$

After simplification (5.46) reduce to ,

$$\begin{aligned} (1 + 2irsin\xi(cos\xi - 1))\hat{u}^{n+1} &= \hat{u}^n \\ (1 + 2iRsin\xi)\hat{v}^{n+1} &= \hat{v}^n \end{aligned} \tag{5.47}$$

and the amplification factors corresponding to (5.47) are given by

$$\rho_B(\xi) = \frac{1}{(1 + 2iRsin\xi)} \qquad \rho_A(\xi) = \frac{1}{(1 + 2irsin\xi(cos\xi - 1))} \tag{5.48}$$

for stability of the solution corresponding to the convection operator it is easily observed that

$$|\rho_B(\xi)| < 1 \tag{5.49}$$

for any value of R.The stability of the solution of the diffusion operator satisfies

$$|\rho_A(\xi)| < \left| \frac{1}{(1 + 2irsin\xi(cos\xi - 1))} \right| < 1 \tag{5.50}$$

for any $r > 0$. Since the solution of (5.27) is represented by the splitting operators, operators are given by (5.59).Therefore the amplification factor corresponding to discrete Fourier transform corresponding to the discretisation of (5.27) is given

$$\rho(\xi) = \rho_A(\xi)\rho_B(\xi) \tag{5.51}$$

and

$$|\rho(\xi)| < |\rho_A(\xi)||\rho_B(\xi)| < 1 \tag{5.52}$$

Therefore the solution of(5.27) using the first order splitting (Lie-Trotter) is unconditionally stable for any positive scalar coefficient of the given operators. □

5.3.3. Algorithm 2 (Second Order Splitting Method)

Over the time interval $[t_n, t_n + \Delta t]$

- Step1

$$u(t_n + \Delta t/2) = e^{(\Delta t/2)A} u(t_n) \text{ with } u(t_n) = u^*(t_n) \tag{5.53}$$

- Step2

$$v(t_n + \Delta t) = e^{\Delta t B} v(t_n) \text{ with } v(t_n) = u(t_n + \Delta t/2) \tag{5.54}$$

- Step3

$$w(t_n + \Delta t/2) = e^{(\Delta t/2)A} w(t_n) \text{ with } w(t_n + \Delta t/2) = v(t_n + \Delta t) \tag{5.55}$$

- Step4

$$u^*(t_n + \Delta t) = w^{(d)}(t_n + \Delta t) \tag{5.56}$$

- Step5 If $T < (n+1)\Delta t$ go to Step1, otherwise stop.

We will be estimated using the Pade' approximation for $e^{\Delta t/2A}$ and $e^{\Delta tB}$, respectively

$$\begin{aligned} e^{(\Delta t/2)A} &= (I - (\Delta t/2)A)^{-1} + O(\Delta t^2) \\ e^{\Delta t B} &= (I - \Delta t B)^{-1} + O(\Delta t^2), \end{aligned} \tag{5.57}$$

Therefore,

$$\begin{aligned} e^{\Delta t(A+B)} &\simeq e^{(\Delta t/2)A} e^{\Delta t B} e^{(\Delta t/2)A} \\ &\simeq (I - (\Delta t/2)A)^{-1}(I - \Delta t B)^{-1}(I - (\Delta t/2)A)^{-1} O(\Delta t^2) \\ &\simeq (I - \Delta t(A+B))^{-1} \end{aligned} \tag{5.58}$$

From the above discussion we could easily observe that,

$$u(t_n + \Delta t) = e^{(\Delta t/2)A} e^{\Delta t B} e^{(\Delta t/2)A} u(t_n) \simeq e^{\Delta t(A+B)} \tag{5.59}$$

The discrete presentation of the Algorithm 2 over the each time interval are as follows:

$$\begin{aligned}
\frac{u_i^{n+1/2} - u_i^n}{\Delta t} &= -\frac{1}{2\Delta x^3}(u_{i+2}^{n+1/2} - 2u_{i+1}^{n+1/2} + 2u_{i-1}^{n+1/2} - u_{i-2}^{n+1/2}) \\
\frac{v_i^{n+1} - v_i^n}{\Delta t} &= \frac{1}{2\Delta x}(v_{i-1}^{n+1} - v_{i+1}^{n+1}) \\
\frac{w_i^{n+1/2} - w_i^n}{\Delta t} &= -\frac{1}{2\Delta x^3}(w_{i+2}^{n+1/2} - 2w_{i+1}^{n+1/2} + 2w_{i-1}^{n+1/2} - w_{i-2}^{n+1/2})
\end{aligned} \tag{5.60}$$

Let $6c\frac{\Delta t}{2\Delta x} = R$ and $\frac{\Delta t}{2\Delta x^3} = r$ Rearranging the terms of (5.43) according to the time level, then

$$\begin{aligned}
ru_{i+2}^{n+1/2} - 2ru_{i+1}^{n+1/2} + 2ru_{i-1}^{n+1/2} - ru_{i-2}^{n+1/2} + u_i^{n+1/2} &= u_i^n \\
-Rv_{i+1}^{n+1} + v_i^{n+1} + Rv_{i-1}^{n+1} &= v_i^n \\
rw_{i+2}^{n+1/2} - 2rw_{i+1}^{n+1/2} + 2rw_{i-1}^{n+1/2} - rw_{i-2}^{n+1/2} + w_i^{n+1/2} &= w_i^n
\end{aligned} \tag{5.61}$$

Next we will investigate the stability analysis for Strang splitting.

5.3.4. Stability Analysis of the Strang Splitting

Theorem 5.2 *For any Δt and Δx The Second Order Splitting Method (Strang Splitting) is stable in ℓ_2 norm.*

Proof For any Δt and Δx Strang Splitting is stable in $\ell 2$ norm.We will consider the Von Neuman stability analysis using the discrete Fourier transform.The discrete Fourier transform (5.61)is given by

$$\begin{aligned}
\hat{u}^n e^{i\xi} &= r\hat{u}^{n+1/2} e^{(i+2)\xi} - 2r\hat{u}^{n+1/2} e^{(i+1)\xi} + 2r\hat{u}^{n+1/2} e^{(i-1)\xi} \\
&\quad + r\hat{u}^{n+1/2} e^{(i-2)\xi} + \hat{u}^{n+1/2} e^{i\xi}
\end{aligned} \tag{5.62}$$

$$\begin{aligned}
\hat{v}^n e^{i\xi} &= -R\hat{v}^{n+1}e^{(i+1)\xi} + \hat{v}^{n+1}e^{i\xi} + R\hat{v}^{n+1}e^{(i-1)\xi} \\
\hat{w}^n e^{i\xi} &= r\hat{w}^{n+1/2}e^{(i+2)\xi} - 2r\hat{w}^{n+1/2}e^{(i+1)\xi} + 2r\hat{w}^{n+1/2}e^{(i-1)\xi} \\
&\quad + r\hat{w}^{n+1/2}e^{(i-2)\xi} - \hat{w}^{n+1/2}e^{i\xi}
\end{aligned}$$

rearanging the terms in (5.62)we get,

$$\begin{aligned}
\hat{u}^n &= (re^{2i\xi} - 2re^{i\xi} + 2re^{-i\xi} - re^{-2i\xi} + 1)\hat{v}^{n+1/2} \\
\hat{v}^n &= (-Re^{i\xi} + 1 + Re^{-i\xi})\hat{u}^{n+1} \\
\hat{w}^n &= (re^{2i\xi} - 2re^{i\xi} + 2re^{-i\xi} - re^{-2i\xi} + 1)\hat{w}^{n+1/2}
\end{aligned} \tag{5.63}$$

After simplification (5.63) reduce to ,

$$\begin{aligned}
(1 + 2irsin\xi(cos\xi - 1))\hat{u}^{n+1/2} &= \hat{u}^n \\
(1 + 2iRsin\xi)\hat{u}^{n+1} &= \hat{u}^n \\
(1 + 2irsin\xi(cos\xi - 1))\hat{w}^{n+1/2} &= \hat{w}^n
\end{aligned} \tag{5.64}$$

and the amplification factors corresponding to (5.64) are given by

$$\rho_B(\xi) = \frac{1}{(1 + 2iRsin\xi)} \qquad \rho_{A/2}(\xi) = \frac{1}{(1 + 2irsin\xi(cos\xi - 1))} \tag{5.65}$$

for stability of the solution corresponding to the operator it is easily observed that

$$|\rho_B(\xi)| < 1 \tag{5.66}$$

for any value of R.The stability of the solution of the diffusion operator satisfies

$$|\rho_{A/2}(\xi)| < |\frac{1}{1 + 2irsin\xi(cos\xi - 1)}| < 1 \tag{5.67}$$

for any $r > 0$. Since the solution of (5.27) is represented by the splitting operators, operators are given by (5.59).Therefore the amplification factor corresponding to discrete

Fourier transform corresponding to the discretisation of (5.27) is given by

$$\rho(\xi) = \rho_{A/2}(\xi)\rho_B(\xi)\rho_{A/2}(\xi) \tag{5.68}$$

and

$$|\rho(\xi)| < |\rho_{A/2}(\xi)||\rho_B(\xi)||\rho_{A/2}(\xi)| < 1 \tag{5.69}$$

Therefore the solution of(5.27) using the second order splitting (Strang Splitting) is unconditionally stable for any positive scalar coefficient of the given operators. □

5.4. General Approach to Von-Neumann Stability Analysis for Operator Splitting Methods

We will investigate the stability of the of the partial differential equations with von Neumann approach. In the approach taken here, it is not necessary to specify a spatial discretisation method. It suffices to know that there exist a spatial discretisation technique that can be applied to the resultant system of equation. Let us consider the linear system of equation,

$$\begin{pmatrix} \partial u/\partial t \\ \partial v/\partial t \end{pmatrix} = \begin{pmatrix} L_1(u) \\ L_2(v) \end{pmatrix} \tag{5.70}$$

where L_1 and L_2 are linear operators $u = u(x,t)$ and $v = v(x,t)$ Suppose that we have a linear map resulting from the application of the 2nd order midpoint rule to the system (5.70) over one time step such that,

$$\begin{pmatrix} u^{'}(x) \\ v^{'}(x) \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} u_0(x) \\ v_0(x) \end{pmatrix} = A^{'} \begin{pmatrix} u_0(x) \\ v_0(x) \end{pmatrix} \tag{5.71}$$

where $A^{'}$ is a matrix of linear operators, $u_0(x) = u(x,t_0)$, $v_0(x) = v(x,t_0)$ are the temporal initial conditions, and $u^{'}(x)$ and $u^{'}(x)$ are the approximations of u and v in function space at time $t = t_0 + \tau$. The stability criterion for the linear map we need to check the eigenvalues of the matrix $A^{'}$. The eigenvalues of the $A^{'}$ are solutions of $\lambda^2 - Tr(A') + det(A') = 0$. Following the stability of the linear maps, if the roots λ_1 and λ_2 of the equation are complex conjugates then,

$$\lambda = \frac{Tr(A')}{2} \pm i\sqrt{det(A') - \left(\frac{Tr(A')}{2}\right)^2} \tag{5.72}$$

with $\mid Tr(A') \mid < 2\sqrt{det(A')}$ and $\lambda \leq 1$. In order to apply stability theory A' must be manipulated into a matrix of scalars. This is done by taking Fourier transforms of (6.1) as would be done in a von-Neumann stability analysis (Regan, 2000). We will restrict this discussion to linear operators that are either spatial derivatives of at least first order or the identity multiplied by real or complex scalars. Given this restriction, applying a continuous Fourier transform to (6.1) according to the formula,

$$\hat{u}(w) = \frac{1}{\sqrt{2\pi}} \int_{\mathbf{R}} e^{-iwx} u(x) dx \tag{5.73}$$

we will yield,

$$\begin{pmatrix} \hat{u}^{'}(w) \\ \hat{v}^{'}(w) \end{pmatrix} = \begin{pmatrix} z_{11}(w) & z_{12}(w) \\ z_{21}(w) & z_{22}(w) \end{pmatrix} \begin{pmatrix} \hat{u}_0(w) \\ \hat{v}_0(w) \end{pmatrix} = A \begin{pmatrix} \hat{u}_0(w) \\ \hat{v}_0(w) \end{pmatrix} \tag{5.74}$$

where $z_{ij}(w)$ are complex scalars involving the frequency $w \in \mathbb{R}$.This gives stability criteria in terms of the spectral variable w.

For Lie-Trotter splitting let take,

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} &= L_1 u \\ \frac{\partial v(x,t)}{\partial t} &= L_2 v \end{aligned} \tag{5.75}$$

where L_1 and L_2 are linear bounded operators. After applying implicit euler method we get,

$$\begin{pmatrix} u'(x) \\ v'(x) \end{pmatrix} = \begin{pmatrix} (I - hL_1)^{-1} & 0 \\ 0 & (I - hL_2)^{-1} \end{pmatrix} \begin{pmatrix} u_0(x) \\ v_0(x) \end{pmatrix} \tag{5.76}$$

Applying a continuous Fourier transform to (5.76) according to formula (5.73) we will yield,

$$\begin{pmatrix} \hat{u}'(w) \\ \hat{u}'(w) \end{pmatrix} = \begin{pmatrix} A_{11}(w) & 0 \\ 0 & A_{22}(w) \end{pmatrix} \begin{pmatrix} \hat{u_0}(w) \\ \hat{u_0}(w) \end{pmatrix} \tag{5.77}$$

where$A_{ij}(w)$ are complex scalars involving the frequency $w \in \mathbb{R}$. This gives stability criteria in terms of the spectral variable w.

For Strang splitting we get,

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} &= L_1 u \\ \frac{\partial v(x,t)}{\partial t} &= L_2 v \\ \frac{\partial w(x,t)}{\partial t} &= L_1 w \end{aligned} \tag{5.78}$$

Application of the second order midpoint rule yields,

$$\begin{pmatrix} u'(x) \\ v'(x) \\ w'(x) \end{pmatrix} = \begin{pmatrix} \frac{I+\frac{hL_1}{2}}{I-\frac{hL_1}{2}} & 0 & 0 \\ 0 & \frac{I+\frac{hL_2}{2}}{I-\frac{hL_2}{2}} & 0 \\ 0 & 0 & \frac{I+\frac{hL_1}{2}}{I-\frac{hL_1}{2}} \end{pmatrix} \begin{pmatrix} u_0(x) \\ v_0(x) \\ w_0(x) \end{pmatrix} \tag{5.79}$$

Taking a Fourier transform of this gives,

$$\begin{pmatrix} \hat{u}'(w) \\ \hat{v}'(w) \\ \hat{w}'(w) \end{pmatrix} = \begin{pmatrix} A_{11}(w) & 0 & 0 \\ 0 & A_{22}(w) & 0 \\ 0 & 0 & A_{33}(w) \end{pmatrix} \begin{pmatrix} \hat{u_0}(w) \\ \hat{v_0}(w) \\ \hat{w_0}(w) \end{pmatrix} \tag{5.80}$$

where $A_{ij}(w)$ are complex scalars involving $w \in \mathbb{R}$. This gives the stability criteria in terms of w.

5.4.1. Stability Analysis of the Lie-Trotter Splitting for Nonlinear KdV Equation

Now in a continuous case we rewrite the equation (5.27) to unbounded operators

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} &= L_1 u \\ \frac{\partial v(x,t)}{\partial t} &= L_2 v \end{aligned} \tag{5.81}$$

where $L_1 = -\frac{\partial^3}{\partial x^3}$ and $L_2 = c\partial x$ with $c = u$ Application of the implicit euler method yields,

$$\begin{pmatrix} u'(x) \\ v'(x) \end{pmatrix} = \begin{pmatrix} \frac{1}{I-hL_1} & 0 \\ 0 & \frac{1}{I-hL_2} \end{pmatrix} \begin{pmatrix} u_0(x) \\ v_0(x) \end{pmatrix} \tag{5.82}$$

Taking a Fourier transform of this gives,

$$\begin{pmatrix} \hat{u}'(x) \\ \hat{v}'(x) \end{pmatrix} = \begin{pmatrix} \frac{1}{1-ihw^3} & 0 \\ 0 & \frac{1}{1-ichw} \end{pmatrix} \begin{pmatrix} \hat{u}_0(x) \\ \hat{v}_0(x) \end{pmatrix} \tag{5.83}$$

For stability it is easily seen that,

$$\lambda_1 = \left| \frac{1}{1-ihw^3} \right| < 1 \quad \text{and} \quad \lambda_2 = \left| \frac{1}{1-ichw} \right| < 1 \tag{5.84}$$

This is true for any choice of w, hence the method is unconditionally stable.

Next, we will apply the same idea for investigating the stability analysis of the nonlinear KdV equation for Strang splitting method.

5.4.2. Stability Analysis of the Strang Splitting for Nonlinear KdV Equation

We have the equation (5.27). We split the equation into two parts and apply the Strang splitting,

$$\begin{aligned}\frac{\partial u(x,t)}{\partial t} &= L_1 u \\ \frac{\partial v(x,t)}{\partial t} &= L_2 v \\ \frac{\partial w(x,t)}{\partial t} &= L_1 w\end{aligned} \tag{5.85}$$

where $L_1 = -\frac{\partial^3}{\partial x^3}$ and $L_2 = c\partial x$ Application of the midpoint rule yields,

$$\begin{pmatrix} u'(x) \\ v'(x) \\ w'(x) \end{pmatrix} = \begin{pmatrix} \frac{I+\frac{hL_1}{2}}{I-\frac{hL_1}{2}} & 0 & 0 \\ 0 & \frac{I+\frac{hL_2}{2}}{I-\frac{hL_2}{2}} & 0 \\ 0 & 0 & \frac{I+\frac{hL_1}{2}}{I-\frac{hL_1}{2}} \end{pmatrix} \begin{pmatrix} u_0(x) \\ v_0(x) \\ w_0(x) \end{pmatrix} \tag{5.86}$$

Taking a Fourier transform of this gives,

$$\begin{pmatrix} \hat{u}'(w) \\ \hat{v}'(w) \\ \hat{w}'(w) \end{pmatrix} = \begin{pmatrix} \frac{1+\frac{ihw^3}{2}}{1-\frac{ihw^3}{2}} & 0 & 0 \\ 0 & \frac{1+\frac{ichw}{2}}{1-\frac{ichw}{2}} & 0 \\ 0 & 0 & \frac{1+\frac{ihw^3}{2}}{1-\frac{ihw^3}{2}} \end{pmatrix} \begin{pmatrix} \hat{u}_0(w) \\ \hat{v}_0(w) \\ \hat{w}_0(w) \end{pmatrix} \tag{5.87}$$

For stability we know that $\lambda_i \leq 1$, $i = 1, 2, 3$

$$\lambda_1 = \left| \frac{1 + \frac{ichw}{2}}{1 - \frac{ichw}{2}} \right| \leq 1 \quad \text{and} \quad \lambda_{2,3} = \left| \frac{1 + \frac{ihw^3}{2}}{1 - \frac{ihw^3}{2}} \right| \leq 1 \tag{5.88}$$

This is true for any choice of w, hence the method is unconditionally stable.

CHAPTER 6

APPLICATIONS OF THE OPERATOR SPLITTING METHODS

This chapter has three main parts. In the first part, traditional operator splitting methods are compared with the proposed higher order methods. For this purpose we solved numerically ODE and PDE problems. Next, we apply the traditional splitting methods to the real life problem (Mathematical model for capillary formation in tumor angiogenesis). Finally, we adapted the traditional operator splitting methods to the non-linear KdV equation.

6.1. Applications of the Higher Order Operator Splitting Methods

In this section, we will apply the traditional and higher operator splitting methods to linear ODE problem and parabolic equation. We will compare the results of the problems and see that we get higher accuracy by accelerating the initial conditions with Zassenhaus products.

6.1.1. Application to Matrix Problem

We first deal with the following linear ordinary differential equation :

$$\frac{\partial u(t)}{\partial t} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} u \tag{6.1}$$

with the initial conditions $u_0 = (1, -1)$ on the interval [0, T]. The analytical solution is given by :

$$u(t) = \begin{pmatrix} e^{-t} \\ e^{t} \end{pmatrix} \tag{6.2}$$

We split our linear operators into two operators by setting:

$$\frac{\partial u(t)}{\partial t} = \begin{pmatrix} 2 & -1 \\ -1 & 0 \end{pmatrix} u + \begin{pmatrix} -2 & 2 \\ 2 & 0 \end{pmatrix} u \tag{6.3}$$

We then have the operators:

$$A = \begin{pmatrix} 2 & -1 \\ -1 & 0 \end{pmatrix} \qquad B = \begin{pmatrix} -2 & 2 \\ 2 & 0 \end{pmatrix} \tag{6.4}$$

For integration constants we use a step size of $\Delta t = 10^{-2}$. We apply the fourth order Runge-Kutta method to our operator splitting schemes with respect to the one operator. We compare the first component of the solution obtained from weighted and without weighted operator splitting schemes with exact solution.

For Lie-Trotter splitting we compare, one term weight we mean with $[A, B] \neq 0$,

$$w_1 = -\frac{1}{2}[A, B]$$

two term weight we mean

$$w_2 = \frac{1}{6}[A, [A, B]] - \frac{1}{3}[B, [B, A]]$$

For Strang splitting we compare the one term weight polynomial,

$$w_1 = \frac{1}{24}[A, [A, B]] - \frac{1}{12}[B, [B, A]]$$

As a first experiment, Lie-Trotter splitting and fourth order Runge-Kutta method is applied with different weight polynomials for $\Delta t = 0.01$. Comparison of the exact solution and the numerical solution of the problem is shown in Figure 6.1. Next, in Figure 6.2 we compare the first component of the solution obtained by Strang splitting with weight and without weighted polynomials for $\Delta t = 0.01$ and fourth order Runge-Kutta method.

The comparison of errors measured by L_∞ and L_1 are given in the Table 6.1 and Table 6.2. The errors used in our computations are calculated by the following equations,

$$err_{L_\infty} := max(max(|u(x_i, t^n) - u_{analy}(x_i, t^n)|)) \tag{6.5}$$

$$err_{L_1} := \sum_{i=1}^{m} \triangle x |u(x_i, t^n) - u_{analy}(x_i, t^n)| \tag{6.6}$$

It can be seen clearly in these tables, the splitting error is reduced by applying weighted polynomials.

Table 6.1. Comparison of errors for $\Delta t = 0.01$.

		err_{L_∞}	err_{L_1}
Lie Trotter Splitting	Without w	0.1194	0.0060
	With one w	0.0292	0.0014
	With two w	0.0284	0.0013

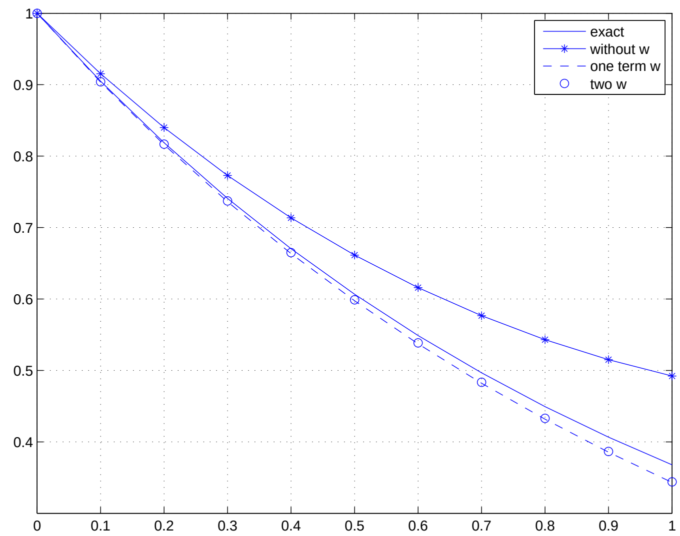

Figure 6.1. Comparison of the solutions of matrix problem obtained by Lie-Trotter splitting.

Table 6.2. Comparison of errors for $\Delta t = 0.01$.

		err_{L_∞}	err_{L_1}
Strang Splitting	Without w	0.0055	2.7104e-004
	With one w	0.0051	2.3562e-004

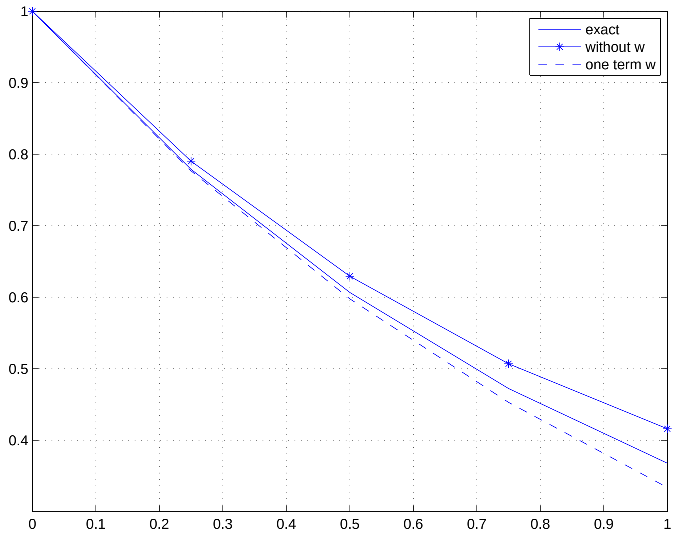

Figure 6.2. Comparison of the solutions of matrix problem obtained by Strang splitting.

6.1.2. Application to Parabolic Equation

We consider a parabolic equation in the following test problem as a next example of higher order splitting method:

$$u_t = Du_{xx}, \tag{6.7}$$

where $(x,t) \in [0,1] \times [0,1]$, $D = \frac{0.5*dx^2}{\sqrt[4]{0.5}}$, with exact solution $u(x,t) = sin(\pi x)e^{-D\pi^2 t}$ and initial conditions are taken from exact solution, boundary conditions are Dirichlet boundary condition.

We shall imply the fourth order difference approximation for u_{xx} as

$$u_{xx} \cong \frac{1}{\Delta x^2}[-1/12 \quad 4/3 \quad -5/2 \quad 4/3 \quad -1/12].$$

Therefore we obtain the first order differential equations given by

$$\frac{du}{dt} = Au, \tag{6.8}$$

where A is the global matrix coefficients given by the following stencil

$$A = \frac{1}{\Delta x^2}[-1/12 \quad 4/3 \quad -5/2 \quad 4/3 \quad -1/12] = A_1 + A_2, \tag{6.9}$$

and $A_1 = (A_l + D)$, $A_2 = A_u$ where A_l is lower triangular matrix, D is Diagonal matrix, A_u is upper triangular matrix.

As a first experiment, Lie-Trotter splitting and implicit Euler method without weight and midpoint rule with one term weight and two weight are applied with different weight polynomials with $\Delta x = 0.1$ and $\Delta t = 0.1$. Comparison of the exact solution and the numerical solution of the problem with different weight polynomials are shown in Figure 6.3. Next, in Figure 6.4 we compare the numerical solution obtained by Strang splitting with weight and without weighted polynomials with $\Delta x = 0.1$ and $\Delta t = 0.1$ and midpoint rule.

The comparison of errors measured by L_∞ and L_1 are given in the Table 6.3 and Table 6.4. It can be is easily seen that we get the same result by using Lie-Trotter with one weight, with Strang Splitting without weight.

Table 6.3. Comparison of errors for $\Delta x = 0.1$ and $\Delta t = 0.1$.

		err_{L_∞}	err_{L_1}
Lie Trotter Splitting	Without w	0.0376	0.0021
	With one w	0.0082	2.1848e-004

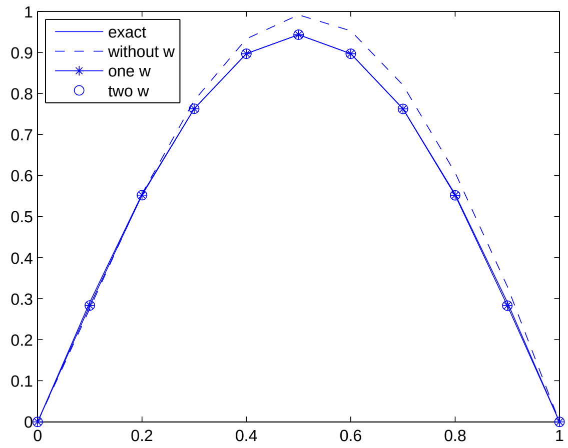

Figure 6.3. Comparison of the solutions of parabolic equation obtained by Lie-Trotter splitting.

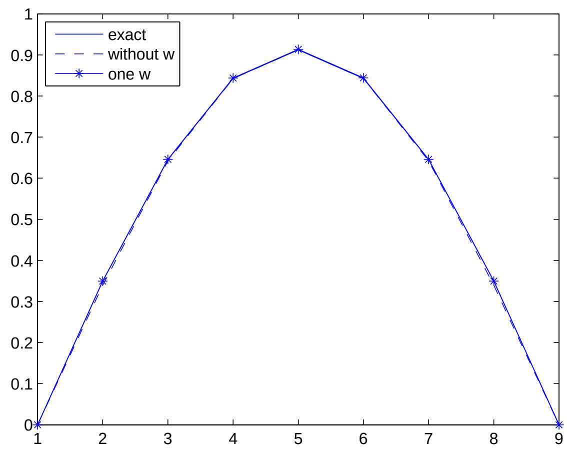

Figure 6.4. Comparison of the solutions of matrix problem obtained by Strang splitting.

Table 6.4. Comparison of errors for $\Delta x = 0.1$ and $\Delta t = 0.1$.

		err_{L_∞}	err_{L_1}
Strang Splitting	Without w	0.0100	4.1548e-004
	With one w	0.0011	8.8875e-005

6.2. Mathematical Model for Capillary Formation in Tumor Angiogenesis

The mathematical model for capillary formation in tumor angiogenesis is originally presented in (Levine et al., 2001). In this model, Levine et al introduces us the following initial boundary value problem and this problem describes the endothelial cell movement in capillary.

$$\frac{\partial u}{\partial t} = D\frac{\partial}{\partial x}(u\frac{\partial}{\partial x}(\ln \frac{u}{f(x)})), \quad x \in (0,1), \quad t \in (0,T] \tag{6.10}$$

Initial condition is given by

$$u(x,0) = 1, \quad x \in (0,1), \tag{6.11}$$

and boundary conditions are given by

$$Du\frac{\partial}{\partial x}(\ln \frac{u}{f(x)}) \mid_0 \;=\; 0, \quad t \in [0,T], \tag{6.12}$$

$$Du\frac{\partial}{\partial x}(\ln \frac{u}{f(x)}) \mid_1 \;=\; 0, \quad t \in [0,T], \tag{6.13}$$

where $f(x)$ is the so-called transition probability function which has the effect of biasing the random walk of endothelial cells and given by

$$f(x) = (\frac{a + A_1 x^k (1-x)^k}{b + A_1 x^k (1-x)^k})^{\alpha_1} (\frac{c + 1 - A_2 x^k (1-x)^k}{d + 1 - A_2 x^k (1-x)^k})^{\alpha_2} \tag{6.14}$$

In this initial boundary value problem (6.10)-(6.13), $u(x,t)$ is the concentration of Endothelial Cells, D is the cell diffusion constant and a, b, c, d, A_1, A_2, k, α_1, α_2 are some arbitrary constants.

Consider the Eq.(6.10), it can be written as

$$D\frac{\partial}{\partial x}(u\frac{\partial}{\partial x}(\ln\frac{u}{f(x)})) = D\frac{\partial}{\partial x}(u(\frac{u'}{u} - \frac{f'(x)}{f(x)})) \tag{6.15}$$

and by setting $F(x) = \frac{f'(x)}{f(x)}$ we have the simplified form

$$u_t = D(u_{xx} - (uF(x))_x). \tag{6.16}$$

The initial condition is

$$u(x,0) = 1, \quad x \in (0,1), \tag{6.17}$$

and boundary conditions (6.12),(6.13) become

$$D(\frac{\partial u}{\partial x} - uF) \mid_0 \;=\; 0 \;\text{ for }\; t > 0, \tag{6.18}$$

$$D(\frac{\partial u}{\partial x} - uF) \mid_1 \;=\; 0 \;\text{ for }\; t > 0, \tag{6.19}$$

We split the equation

$$u_t = D(u_{xx} - u_x F - F_x u) \tag{6.20}$$

into two parts as follows: Diffusion part is

$$u_t = Du_{xx} \tag{6.21}$$

and advection-reaction part is

$$u_t = -Du_xF - DF_xu. \tag{6.22}$$

For initial condition we have

$$u_m = 1, \quad 0 \leq m \leq N, \tag{6.23}$$

and for boundary conditions (6.18), (6.19), we have

$$D(\frac{\partial u_0}{\partial x} - u_0F_0) = 0, \text{ for } t > 0, \tag{6.24}$$
$$D(\frac{\partial u_N}{\partial x} - u_NF_N) = 0, \text{ for } t > 0 \tag{6.25}$$

where m defines the spatial discretisation step and N is the spatial discretisation number. The derivatives terms in Eqs. (6.24), (6.25) are approximated by using the the backward and forward difference formulas. Next, the central difference approximation for each derivative terms u_{xx} and u_x are taken into account as follows: Diffusion term at each grid point (x_m, t) becomes

$$\frac{\partial^2 u}{\partial x^2} \mid_{(x_m,t)} = \frac{1}{h^2}(u_{m+1}(t) - 2u_m(t) + u_{m-1}(t)) \tag{6.26}$$

and advection term at each grid point (x_m, t) becomes

$$\frac{\partial u}{\partial x} \mid_{(x_m,t)} = \frac{1}{2h}(u_{m+1}(t) - u_{m-1}(t)) \tag{6.27}$$

where h is the spatial stepping and $m = 0, 1, \ldots, N$.

After assembling the unknowns of (6.26), for each m, and embedding the approximation of derivative terms in boundary conditions in (6.24), (6.25), we have the following system of equations in matrix form as follows:

$$u_{xx} = A_1 u \tag{6.28}$$

where

$$A_1 = \frac{1}{h^2}\begin{pmatrix} -2+(1-hF_0) & 1 & 0 & \dots & 0 & 0 \\ 1 & -2 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \dots & \vdots & 0 \\ 0 & 0 & 0 & \dots & -2 & 1 \\ 0 & 0 & 0 & \dots & 1 & -2+(1+hF_N) \end{pmatrix} \tag{6.29}$$

A_1 is $(N+1)\times(N+1)$ matrix and by assembling the unknowns of (6.27), for each m, we obtain the following system

$$u_x = B_1 u \tag{6.30}$$

where

$$B_1 = \frac{1}{2h}\begin{pmatrix} -(1-hF_0) & 1 & 0 & \dots & 0 & 0 \\ -1 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \dots & \vdots & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 0 & \dots & -1 & (1+hF_N) \end{pmatrix} \tag{6.31}$$

B_1 is $(N+1)\times(N+1)$ matrix.

We fix the functions $F(x)$ and $F'(x)$ at each discretisation points $m = 0, 1, \dots, N$

and have

$$F(\underline{x}) = \begin{pmatrix} F(x_0) & 0 & \dots & 0 \\ 0 & F(x_1) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & F(x_N) \end{pmatrix} \tag{6.32}$$

and

$$F'(\underline{x}) = \begin{pmatrix} F'(x_0) & 0 & \dots & 0 \\ 0 & F'(x_1) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & F'(x_N) \end{pmatrix} \tag{6.33}$$

where we use central difference approximation for each $F'(x_m)$.

We finally get,

$$u_t = (A + B)u \tag{6.34}$$

where $A = DA_1$, $B = -DF(\underline{x})B_1 - DF'(\underline{x})$.

For numerical computation we consider the problem (6.10)-(6.13) with parameters $D = 0.00025$, $a = 1$, $b = 2$, $c = 10$, $d = 0.1$, $\alpha_1 = \alpha_2 = 1$, $A_1 = 28 \times 10^7$, $A_2 = 0.22 \times 10^9$ and $k = 16$. We write the computer program in matlab and present our results on graphs which are taken at different times.

Numerical solution of the problem (6.10)-(6.13) by using Lie-Trotter splitting, Strang splitting and Symmetrically weighted splitting are given in Figure 6.5, Figure 6.6 and Figure 6.7.Figures show similar trends as ones that obtained by method of lines (Pamuk & Erdem, 2007) and exponentially-fitted method (Erdoğan et al., 2009).

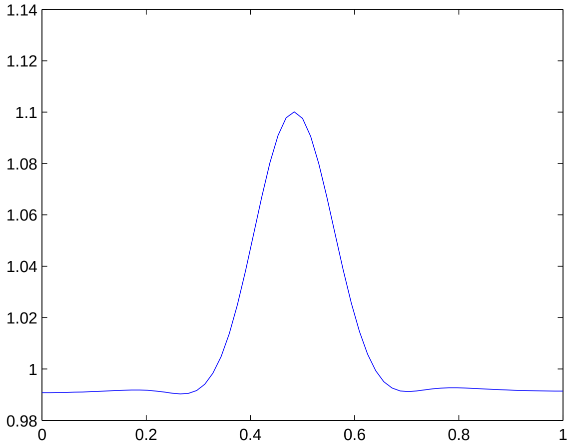

Figure 6.5. Numerical solution of the problem by using Lie-Trotter splitting method for $T = 750$.

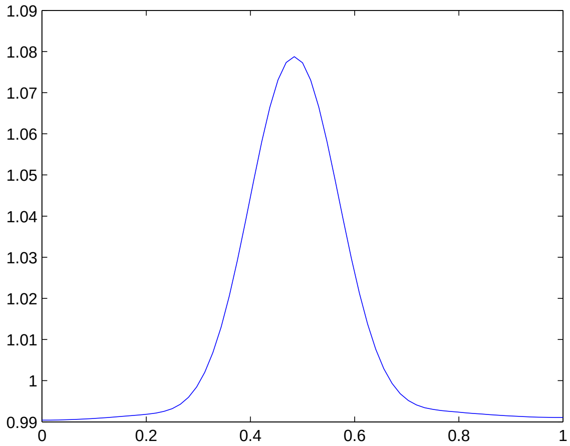

Figure 6.6. Numerical solution of the problem by using Strang splitting method for $T = 750$.

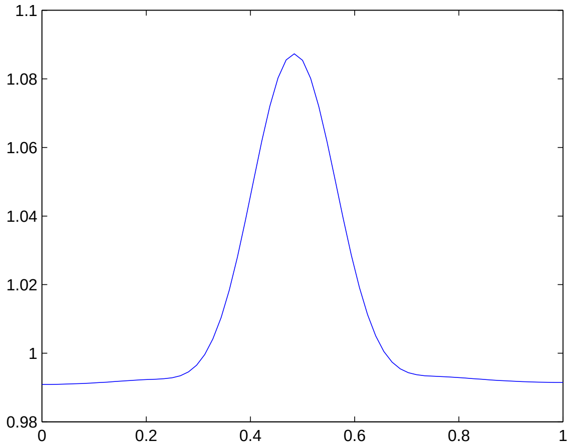

Figure 6.7. Numerical solution of the problem by using Symmetrically weighted splitting method for $T = 750$.

6.3. Nonlinear KdV Equation

We consider the nonlinear KdV equation,

$$U_t - 6UU_x + U_{xxx} = 0 \tag{6.35}$$

which models Russell's observation. The term UU_x describes the sharpening of the wave and U_{xxx} the dispersion. Let $x_i = i\Delta x$ and $t_n = n\Delta t, \quad i = 1, ..., M-1 \;\; n = 0, ..., N$ Respectively $\Delta x = \frac{1}{M}$ $\Delta t = \frac{1}{N}$ are the regular spatial end time step sizes. The first step towards solving is to consider the fractional splitting method, which can be expressed as follows:

$$u_t = -u_{xxx}, \quad [t_n, t_n + \Delta t], \tag{6.36}$$

$$v_t = 6uv_x, \quad [t_n, t_n + \Delta t], \quad v(t_n) = u(t_n + \Delta t) \tag{6.37}$$

We substitute the solution of the equation (6.36) for u in (6.37), We imply the semi-discretisation for (6.35) using the central difference approximation. The finite difference approximation of the operators (6.35) are given by,

$$u_t = Au \tag{6.38}$$

$$v_t = Bv \tag{6.39}$$

where A and B are global matrices of coefficients resulting from the discretisation of $-u_{xxx}$ and v_x

$$A = -\frac{1}{2\Delta x^3}[1 \quad -2 \;\; 2 \quad -1] \tag{6.40}$$

$$B = 6c_i\frac{1}{2\Delta x}[-1 \;\; 0 \;\; 1] \tag{6.41}$$

where $c_i = u_i$

The one -soliton solution is given by

$$u(x,t) = -\frac{v}{2\cosh^2(\frac{1}{2}\sqrt{v}(x - vt))} \tag{6.42}$$

and the parameter v is taken as $v = 16$.

For the first experiment, the one soliton solution of the KdV equation is obtained by Strang splitting and Runge-Kutta method. We solved the problem in the region $-8 \leq x \leq 8$ with a grid size $\Delta x = 0.1$ and $\Delta t = 0.1$. The periodic boundary conditions are chosen. The comparison of the exact solution and numerical solution of the KdV equation at fixed $t = 2$ is shown in Figure 6.8.

Next, Lie-Trotter splitting and Runge-Kutta are also implemented to obtain one soliton solution of the KdV equation. The comparison of errors measured by L_∞ and L_1 are given in the Table 6.5.

It can be seen clearly in this table, second order Strang splitting method can achieve more accurate result than Lie-Trotter splitting method. The proposed algorithms are efficient to find the approximated solution for the model problem, as we expected from our stability analysis.

Table 6.5. Comparison of errors for $h = 0.1$.

	err_{L_∞}	err_{L_1}
Lie-Trotter Splitting	0.1707	0.0358
Strang Splitting	0.0954	0.0132

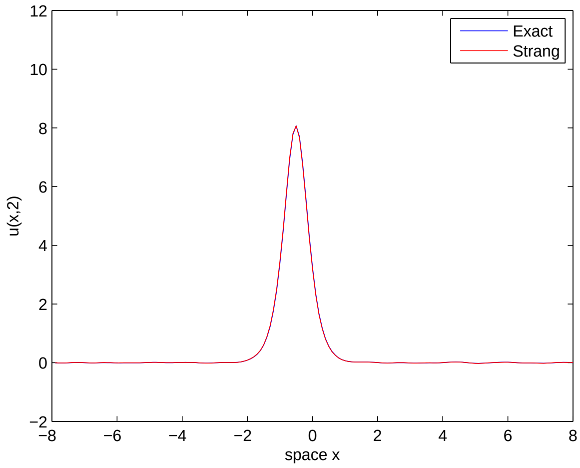

Figure 6.8. Numerical solution of one-soliton for h=0.1 and fixed t=2. The dashed line indicates the exact solution.

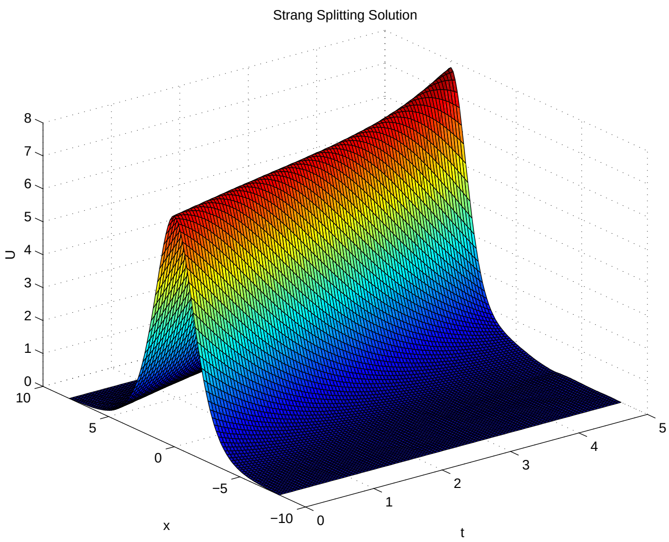

Figure 6.9. Numerical solution of one-soliton case for h=0.1 and up to t=5.

CHAPTER 7

CONCLUSION

In this thesis, we introduced the traditional operator splitting methods; Lie-Trotter splitting, additive splitting, symmetrically weighted splititng, Strang splitting and higher order splitting methods which are obtained by the Zassenhaus product formula. Consistency analysis for linear bounded operators are studied by the means of Zassenhaus product formula and for unbounded operators by C_0-semigroup approach. We derived the algorithms for the nonlinear KdV equation and studied the stability analysis for these operator splitting methods. We reformulated to Von-Neumann stability analysis for Lie-Trotter and Strang splitting. We extend the operator splitting methods to solve various ODEs and PDEs.

Starting with the traditional and proposed operator splitting methods are applied to matrix problem. For that problem we observed that, the splitting error reduced by applying weighted polynomials. We get the same result by using Lie-Trotter splitting with one weight, with Strang splitting without weight. So, proposed operator splitting methods lead us advantage for the CPU times.

Next, we applied the operator splitting methods to real life problem (mathematical model for capillary formation in tumor angiogenesis). The graphs in 6.5, 6.6 and 6.7 show similar trends as the ones that obtained by method of lines and exponentially fitted method.

Finally, we adapted the traditional splitting methods to nonlinear KdV equation. This adaptation leads us to use Von-Neumann stability analysis for the proposed methods. We presented the errors obtained by Lie-Trotter and Strang splitting measured by L_∞ and L_1 are given in the Table 6.5. Results give us proposed algorithms work and expected order of the accuracy for the operator splitting methods are confirmed.

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APPENDIX A

MATLAB CODES FOR THE APPLICATIONS OF THE OPERATOR SPLITTING METHODS

HIGHER ORDER AND TRADITIONAL OPERATOR SPLITTING METHODS MATLAB CODE FOR MATRIX PROBLEM

```
%Lie-Trotter splitting for matrix problem
Nt=10; A=[2 -1 ; -1 0]; B=[-2 2; 2 0];
u11=zeros(2,Nt+1);  u22=zeros(2,Nt+1);  u33=zeros(2,Nt+1);
u11(:,1)=[1;-1];    u22(:,1)=[1;-1];    u33(:,1)=[1;-1];
uini1=[1;-1];       uini2=[1;-1];       uini3=[1;-1];
T=1;t0=0;           dt=(T-t0)/Nt
C=(B*A-A*B);        D=(B*C-C*B);
E=A*(A*B-B*A)-(A*B-B*A)*A;
W1=eye(size(B))-(1/2)*C*dt^2;
W2=eye(size(B))-(1/2)*C*dt^2+((1/6)*D-(1/3)*E)*dt^3;
t=t0:dt:T;
for i=1:(Nt+1)
ye(i)=exp(-t(i));
end
for s=2:Nt+1,
u1=runfour(A,uini1,dt);
v1=u1;
u1=runfour(B,v1,dt);
uini1=u1;
u11(:,s)=u1;
u2=runfour(A,uini2,dt);
v2=W1*u2;
u2=runfour(B,v2,dt);
uini2=u2;
u22(:,s)=u2;
u3=runfour(A,uini3,dt);
v3=W2*u3;
```

```
u3=runfour(B,v3,dt);
uini3=u3;
u33(:,s)=u3;
end
u11(1,:);     u22(1,:);        u33(1,:)
plot(t,ye);hold on;plot(t,u11(1,:),'*-');
hold on;plot(t,u22(1,:),'--');
hold on;plot(t,u33(1,:),'o');grid on;
legend('exact','without w','one term w','two w');
e1 = max(max(abs(ye-u11(1,:))))
e2=dt^2*sum(sum(abs(ye-u11(1,:))))
errweight1 = max(max(abs(ye-u22(1,:))))
errweight2=dt^2*sum(sum(abs(ye-u22(1,:))))
errweight11 = max(max(abs(ye-u33(1,:))))
errweight21=dt^2*sum(sum(abs(ye-u33(1,:))))
%Strang splitting for matrix problem
Nt=10;
A=[2 -1 ; -1 0];
B=[-2 2; 2 0];
u11=zeros(2,Nt+1);  u22=zeros(2,Nt+1);  u33=zeros(2,Nt+1);
u11(:,1)=[1;-1];    u22(:,1)=[1;-1];    u33(:,1)=[1;-1];
uini1=[1;-1];       uini2=[1;-1];       uini3=[1;-1];
T=1;t0=0;           dt=(T-t0)/Nt
C=(B*A-A*B);        D=(B*C-C*B);
E=A*(A*B-B*A)-(A*B-B*A)*A;
W1=eye(size(B))-((1/24)*D+(1/12)*E)*dt^3;
for i=1:(Nt+1)
ye(i)=exp(-t(i));
end
for s=2:Nt+1,
dtt=dt/2;
u1=runfour(A,uini1,dtt);     v1=u1;
u1=runfour(B,v1,dt);         v2=u1;
u1=runfour(A,v2,dtt);        uini1=u1;
u11(:,s)=u1;
```

```
u2=runfour(A,uini2,dtt);    p2=W1*u2;
u2=runfour(B,p2,dt);        m2=u2;
u2=runfour(A,m2,dtt);       uini2=u2;
u22(:,s)=u2;
u11(1,:);    u22(1,:);
plot(t,ye);hold on;plot(t,u11(1,:),'*-');
hold on;plot(t,u22(1,:),'--');grid on;
legend('exact','without w','one term w');
function fun=runfour(A,x0,dt);
x=zeros(2,2);
x(:,1)=x0;
for i=2:2
k1=dt*fli(A,x(:,i-1));
k2=dt*fli(A,x(:,i-1)+k1/2);
k3=dt*fli(A,x(:,i-1)+k2/2);
k4=dt*fli(A,x(:,i-1)+k3);
x(:,i)= x(:,i-1)+(k1+2*k2+2*k3+k4)/6;
end  fun=x(:,2);
```

HIGHER ORDER AND TRADITIONAL OPERATOR SPLITTING METHODS

MATLAB CODE FOR PARABOLIC PROBLEM

```
%%%%%% Lie-Trotter splitting for parabolic problem
xp=0;X=1;tp=0;T=1;N=10;Nt=10;
dx=1/N;dt=1/Nt;x=xp:dx:X;t=tp:dt:T;
D=(0.5*dx^2)/(0.5)^(1/4);
k=dt^2;
%%%exact solution
for i=1:N
for j = 1:Nt+1
exact(i,j) = sin(pi*x(i))*exp(-D*pi^(2)*t(j));
end end
%% initail conditon
for i = 1 : N+1
x0(i) = sin(pi*x(i))*exp(-D*pi^(2)*t(1));
x01(i) = sin(pi*x(i))*exp(-D*pi^(2)*t(1));
x02(i) = sin(pi*x(i))*exp(-D*pi^(2)*t(1)); end
```

```
x0=x0'
sin(pi*x(N))*exp(-D*pi^(2)*t(1));
sin(pi*x(N))*exp(-D*pi^(2)*t(2));
sin(pi*x(N))*exp(-D*pi^(2)*t(3));
%% boundary conditons
for j = 1 : Nt+1
xbl(j) = 0; xbr(j) = 0;  end
for i=1
for j = 1:Nt+1
exact(i,j) = 0; end end
%% definition of B 4th order% -1/12 4/3 -5/2 4/3 -1/12
n=N-2;  B=toeplitz([-5/2 4/3 -1/12 0   zeros(1,n-1)],
[-5/2 4/3 -1/12 0 zeros(1,n-1)]);
full(B);  B = D/(dx^2)*B;
B(1,1)=0; B(1,2)=0; B(1,3)=0;
B(N+1,N+1)=0;B(N+1,N)=0; B(N+1,N-1)=0;
full(B);
B1=zeros(N+1,Nt+1);
B2=zeros(N+1,Nt+1);
%%%%%%%%%% B1 %%%%%%%%%%%
n=N-2;  B1=toeplitz([-5/2 0 0 0   zeros(1,n-1)],
[-5/2 4/3 -1/12 0 zeros(1,n-1)]);
full(B1); B1 = D/(dx^2)*B1;
B1(1,1)=0; B1(1,2)=0; B1(1,3)=0;
B1(N+1,N+1)=0;B1(N+1,N)=0; B1(N+1,N-1)=0;
full(B1);
% %%%%%%%%%%%%%%% B2  %%%%%%%%%%%%%%%%
n=N-2;  B2=toeplitz([0 4/3 -1/12 0   zeros(1,n-1)],
[0 0 0 0 zeros(1,n-1)]);
full(B2);  B2 = D/(dx^2)*B2;
B2(1,1)=0; B2(1,2)=0; B2(1,3)=0;
B2(N+1,N+1)=0;B2(N+1,N)=0; B2(N+1,N-1)=0;
full(B2); M=B1+B2
C=(B2*B1-B1*B2)
D=(B2*C-C*B2);
```

```
E=(B1*(B1*B2-B2*B1)-(B1*B2-B2*B1)*B1);
w1=eye(size(B2))-(1/2)*C*dt^2;
w2=eye(size(B2))-(1/2)*C*dt^2+((1/6)*D-(1/3)*E)*dt^3;
ni = [1,2,3];  for j = 1: length(ni)
ua= zeros(N+1,Nt+1,j); ua1=zeros(N+1,Nt+1,j);
ua2=zeros(N+1,Nt+1,j); end for i = 1: length(ni)
ua(:,1,i)= x0'; ua(1,:,i)= xbl(i);
ua(end,:,i)=xbr(i); ua1(:,1,i)= x0';
ua1(1,:,i)= xbl(i); ua1(end,:,i)=xbr(i);
ua2(:,1,i)= x0'; ua2(1,:,i)= xbl(i);
ua2(end,:,i)=xbr(i); end  m=1;  v=2;
for a=1:Nt
erg(:,:,v) = NUM3p(B1,x0,dt,Nt,N,m,a);
v1=erg(:,a+1,v);
erg(:,:,v)=NUM3p(B2,v1,dt,Nt,N,m,a);
usp=erg(:,a+1,v);
x0=usp;  ua(:,a+1,v)=usp;
erg1(:,:,v) = NUM3p(B1,x01,dt,Nt,N,v,a);
v11=w1*erg1(:,a+1,v);
erg1(:,:,v)=NUM3p(B2,v11,dt,Nt,N,v,a);
usp1=erg1(:,a+1,v);
x01=usp1;   ua1(:,a+1,v)=usp1;
erg2(:,:,v) = NUM3p1(B1,x02,dt,Nt,N,v,a);
v12=w2*erg1(:,a+1,v);
erg2(:,:,v)=NUM3p1(B2,v12,dt,Nt,N,v,a);
usp2=erg2(:,a+1,v);
x02=usp2;  ua2(:,a+1,v)=usp2;      end
uaa=ua(:,:,v); uaa1=ua1(:,:,v);  uaa2=ua1(:,:,v);
uaa(N+1,:)=0; uaa1(N+1,:)=0;   uaa2(N+1,:)=0;
plot(x,exact(:,end));hold on;  plot(x,uaa(:,end),'--');
hold on;   plot(x,uaa1(:,end),'-*');
hold on;plot(x,uaa2(:,end),'o');
legend('exact','without w','one w','two w',2);
function erg2 = NUM3p(C,x0,dt,Nt,N,k,a)
u1= zeros(N+1,Nt+1);
```

```
u2= zeros(N+1,Nt+1);  u3= zeros(N+1,Nt+1);
u1(:,a)= x0';   u2(:,a)= x0';   u3(:,a)= x0';
b=a+1; if k==1 for  i=b:b
u1(:,i)= (eye(size(C))-dt*C) \ (u1(:,i-1));
u(1,i)= xbb;   end
erg2=u1; else if k==2    for  ii=b:b
C1= (eye(size(C))-(dt/2)*C);
C2=  (eye(size(C))+ (dt/2)*C);
u2(:,ii)=  C1 \(C2*u2(:,ii-1));  u(1,i)= xbb;
end   erg2=u2;  else if k==3   for  ij=b:b
u11= u3(:,ij-1);  a1= feval('runge',C,u11);
a2=feval('runge',C,u11+(dt/2)*a1);
a3=feval('runge',C,u11+(dt/2)*a2);
a4=feval('runge',C,u11+dt*a3);
u3(:,ij)= u3(:,ij-1)+(dt/6)*(a1+2*a2+2*a3+a4);
u(1,i)= xbb;  end   erg2=u3;
end    end    end
%%%%%% Strang splitting for parabolic problem"
C=(B1*B2-B2*B1);
D=(B2*C-C*B2);
E=(B1*(B2*B1-B1*B2)-(B2*B1-B1*B2)*B1);
w1=eye(size(B2))+(1/24)*D*dt^3-(1/12)*E*dt^3;
v=2; m=2; for a=1:Nt
dtt=dt/2;
erg(:,:,v) = NUM3p(B1,x0,dtt,Nt,N,m,a);
v1=erg(:,a+1,v);
erg(:,:,v)=NUM3p(B2,v1,dt,Nt,N,m,a);
v2=erg(:,a+1,v)
erg(:,:,v) = NUM3p(B1,v2,dtt,Nt,N,m,a);
usp=erg(:,a+1,v);
x0=usp;
ua(:,a+1,v)=usp;
end uaa=ua(:,:,v);
uaa1=ua1(:,:,v);exact(N+1,:)=0;
uaa(N+1,:)=0;uaa1(N+1,:)=0;
```

```
plot(exact(:,end));hold on;
plot(uaa(:,end),'--');hold on;
plot(uaa1(:,end),'-*');
legend('exact','without w','one w',2);
e1 = max(max(abs(uaa(:,end)-exact(:,end))))
e2=dx^2*sum(sum(abs(uaa(:,end)-exact(:,end))))
errweight1 = max(max(abs(uaa1(:,end)-exact(:,end))))
errweight2=dx^2*sum(sum(abs(uaa1(:,end)-exact(:,end))))
```

OPERATOR SPLITTING METHODS MATLAB CODE FOR PARABOLIC PROBLEM CAPILLARY FORMATION in TUMOR ANGIOGENESIS

```
%with Lie-Trotter splitting
N=64; M=50; x0=0; xl=1;
t0=0; T=500; dx=(xl-x0)/N;
dt=(T-t0)/M; D=0.00025;
r=D*dt/(dx)^2;
r2=D*dt/2*dx;
x=x0:dx:xl+2*dx;
t=t0:dt:T;
% %%%%%%% diffusion part   matrix for u1'=D*A1*u1
n=N-2; A1=toeplitz([-2 1 0 0  zeros(1,n-1)],
[-2 1 0 0  zeros(1,n-1)]);
full(A1);
size(A1);
Aa=zeros(N+1);
Aa(1,1)=(1-(fu(x(2))-fu(x(1)))/fu(x(1)));
Aa(N+1,N+1)=(1+(fu(x(N+1))-fu(x(N)))/fu(x(N+1)));
A1=(A1+Aa);
A1=(1/((dx)^2))*A1;
A=D*A1;
size(A);
% %%%%%% convection part %%%%%%
A2=toeplitz([0 -1 0 0    zeros(1,n-1)]
,[0 1 0 0  zeros(1,n-1)]);
full(A2);
Aa2=zeros(N+1);
```

```
Aa2(1,1)=-(1-(fu(x(2))-fu(x(1)))/fu(x(1)));
Aa2(N+1,N+1)=(1+(fu(x(N+1))-fu(x(N)))/fu(x(N+1)));
A2=D*(1/(2*dx))*(A2+Aa2);
A2;
% % %%%%%% matrixes for F(xi) %%%%%%%%%
Ff=zeros(N+1);
for i=1:N+1,
Ff(i,i)=(fu(x(i+1))-fu(x(i)))/(dx*fu(x(i)));
end Ff; Ff=D*A2*Ff;
% %%%%% matrixes for F(xi)derivative %%%%%%%%%%
Ffd=zeros(N+1);
for i=1:N+1,
Ffd(i,i)=((fu(x(i+2))-2*fu(x(i+1))+
fu(x(i)))*fu(x(i))/(dx^2)-((fu(x(i+1))-
fu(x(i)))^2)/(dx^2))/(fu(x(i)))^2;
end Ffd=D*Ffd;
B=-(Ff+Ffd);
% % % % % %%%%%%% initial conditions %%%
for i = 1 : N+1 x0(i) =1;
end x0=x0';
ni = [1,2,3];
for j = 1: length(ni)
ua= zeros(N+1,M+1,j);
end for i = 1: length(ni)
ua(:,1,i)= x0';end
m=1;v=2;
for a=1:M
erg(:,:,v) = tum(A,x0,dt,M,N,m,a);
v1=erg(:,a+1,v);
erg(:,:,v)=tum(B,v1,dt,M,N,m,a);
usp=erg(:,a+1,v);
x0=usp;
ua(:,a+1,v)=usp;
end uaa=ua(:,:,v);
s=0:dx:xl;
```

```
plot(s,uaa(:,end))
%% with Strang splitting
ni = [1,2,3];
for j = 1: length(ni)
ua= zeros(N+1,M+1,j);
end
for i = 1: length(ni)
ua(:,1,i)= x0';
end m=1; v=2;
for a=1:M
dtt=dt/2;
erg(:,:,v) = tum(A,x0,dtt,M,N,m,a);
v1=erg(:,a+1,v);
erg(:,:,v)=tum(B,v1,dt,M,N,m,a);
v2=erg(:,a+1,v);
erg(:,:,v) = tum(A,v2,dtt,M,N,m,a);
usp=erg(:,a+1,v);
x0=usp;
ua(:,a+1,v)=usp;
uaa=ua(:,:,v);
s=0:dx:xl;
plot(s,uaa(:,end))
%with Symmetrically weighted splitting
ni = [1,2,3];
for j = 1: length(ni)
ua= zeros(N+1,M+1,j);
ua1= zeros(N+1,M+1,j);
end
for i = 1: length(ni)
ua(:,1,i)= x0';
ua1(:,1,i)= x01';
end m=1; v=2;
for a=1:M
erg(:,:,v) = tum(A,x0,dt,M,N,m,a);
v1=erg(:,a+1,v);
```

```
erg(:,:,v)=tum(B,v1,dt,M,N,m,a);
usp=erg(:,a+1,v);
x0=usp;
ua(:,a+1,v)=usp;
erg2(:,:,v) = tum(B,x01,dt,M,N,m,a);
v2=erg(:,a+1,v);
erg2(:,:,v)=tum(A,v2,dt,M,N,m,a);
usp1=erg2(:,a+1,v)
x01=usp1;
ua1(:,a+1,v)=usp1;
end
uaa=ua(:,:,v);
uaa1=ua1(:,:,v);
uaaa=(uaa+uaa1)/2;
s=0:dx:xl;
plot(s,uaaa(:,end))
function erg2 = tum(C,x0,dt,M,N,k,a)
u1= zeros(N+1,M+1);
u2= zeros(N+1,M+1);
u3= zeros(N+1,M+1);
u1(:,a)= x0';u2(:,a)= x0';
u3(:,a)= x0'; b=a+1;
if k==1 for  i=b:b
u1(:,i)= (eye(size(C))-dt*C)\(u1(:,i-1));
end erg2=u1;
else if k==2
for  ii=b:b
C1= (eye(size(C))-(dt/2)*C);
C2=  (eye(size(C))+ (dt/2)*C);
u2(:,ii)=  C1 \(C2*u2(:,ii-1));
end erg2=u2;
else if k==3
for  ij=b:b
u11= u3(:,ij-1);
a1= feval('runge',C,u11);
```

```
a2=feval('runge',C,u11+(dt/2)*a1);
a3=feval('runge',C,u11+(dt/2)*a2);
a4=feval('runge',C,u11+dt*a3);
u3(:,ij)= u3(:,ij-1)+(dt/6)*(a1+2*a2+2*a3+a4);
end erg2=u3;
end end end
SPLITTING METHODS MATLAB CODE FOR NONLINEAR KdV
%%Soliton with Lie-Trotter
function solitona
h=0.1;
x=(-8+h:h:8)';
m=length(x);
k=h^3;
n=2/k;
u=firstsol(x,16,0);
for i=1:n
a11=k*f1(u); a21=k*f1(u+a11/2);
a31=k*f1(u+a21/2); a41=k*f1(u+a31);
u=u+a11/6+a21/3+a31/3+a41/6;
a1=k*f2(u); a2=k*f2(u+a1/2);
a3=k*f2(u+a2/2); a4=k*f2(u+a3);
u=u+a1/6+a2/3+a3/3+a4/6;
end
plot(x,-u);
axis([-8,8,-2,12])
xlabel('space x')
ylabel('u(x,2)')
function dudt=f1(u)
u = [u(end-1:end); u; u(1:2)]; h=.1;
dudt = -(u(5:end)-2*u(4:end-1)+
2*u(2:end-3)-u(1:end-4))/2/h^3;
function dudt=f2(u)
u = [u(end-1:end); u; u(1:2)]; h=.1;
dudt = 6*(u(3:end-2)).*(u(4:end-1)
-u(2:end-3))/2/h;
```

```
function u=firstsol(x,v,x0)
u=-v/2./cosh(.5*sqrt(v)*(x-x0)).^2;
%%% Soliton wiith strang Splitting
function solitonst
a11=s*f1(u); a21=s*f1(u+a11/2);
a31=s*f1(u+a21/2); a41=s*f1(u+a31);
u=u+a11/6+a21/3+a31/3+a41/6;
a1=k*f2(u); a2=k*f2(u+a1/2);
a3=k*f2(u+a2/2); a4=k*f2(u+a3);
u=u+a1/6+a2/3+a3/3+a4/6;
a12=s*f1(u); a22=s*f1(u+a12/2);
a32=s*f1(u+a22/2); a42=s*f1(u+a32);
u=u+a12/6+a22/3+a32/3+a42/6;
end
plot(x,-u1); hold on;
plot(x,-u,'r');
axis([-8,8,-2,12])
xlabel('space x')
ylabel('u(x,2)')
```