Operator Splitting Methods: Numerical Solutions of Ordinary Differential Equations via Separation of Variables

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Abstract. This paper applies the concept of linear semigroups induced by nonlinear flows, originally developed by Dorroh and Neuberger in the 1990s, to the approximation of uniquely solvable initial value problems for nonlinear ordinary differential equations. Building on a framework rooted in the earlier works of Lie, Kowalewski, and Gröbner, we analyze nonlinear systems through the lens of the Koopman–Lie semigroup $e^{t\mathcal{K}}$, where $\mathcal{K}$ is the (linear) Lie generator associated with the flow induced by the (nonlinear) differential equation. A central feature of this approach is the decomposition $\mathcal{K} = \mathcal{K}_1 + \cdots + \mathcal{K}_N$, which enables the use of operator splitting methods. We revisit the foundational first-order splitting scheme introduced by H. F. Trotter in 1959 and extend it to higher-order schemes with improved error bounds. Theoretical developments are supported by numerical examples demonstrating the accuracy and efficiency of these methods, based entirely on the classical separation of variables technique, for solving ordinary differential equations.

Key words. Flows, Koopman semigroups, Lie generators, strongly continuous and bi-continuous semigroups, Chernoff's product formula, exponential splitting, higher-order splitting.

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1. Introduction.

Towards the end of the 19th century, several scientists highlighted the impossibility of precisely determining the state of every particle (position or momentum) within a gas or fluid. Notable figures in this development include Boltzmann [7, 8], Gibbs [20, 21], and Poincaré [47, 48]. This insight made it clear that understanding the evolution of macroscopic quantities, such as temperature and pressure, over time was essential. This shift in focus contributed to the development of an alternative framework for dynamical systems, based on the concept of the dynamics of observables, a framework later formalized in quantum mechanics by Heisenberg [28], Dirac [12], and von Neumann [58].

A key element within this framework is the Koopman-Lie operator, a linear operator that effectively captures the dynamics of observations within a dynamical system. By encoding the evolution of observable functions along the trajectories of dynamical systems, the Koopman-Lie operator provides a global linearization of nonlinear systems. This approach enables the study of nonlinear dynamical systems using the tools of linear mathematics, offering a powerful framework for analyzing complex dynamics (see [30] and [32]).

Kowalewski [34] demonstrates that Lie had already employed the concept of flow semigroups and their generators, referred to as Lagrange operators, in his study of ordinary differential equations

$$x'(t) = F(x(t)), \quad x(0) = x_0 = x \tag{1.1}$$

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where $F = (F_1, \ldots, F_N)$ and $F_i : \mathbb{R}^N \supset \Omega \to \mathbb{R}$. To further emphasize Lie's foundational contributions to the framework later developed by Koopman, we will henceforth name key elements of the resulting theory (flows and their generators) after both Koopman and Lie.

Koopman's 1931 work [30] was central to the celebrated proofs of the ergodic theorem by von Neumann [59] and Birkhoff [4, 5]. Koopman introduced his operator theoretic perspective of dynamical systems in 1931 to describe the evolution of measurements of Hamiltonian systems [31], Koopman drew connections between the Koopman eigenvalue spectrum and conserved quantities, integrability, and ergodicity. This theory was generalized by Koopman and von Neumann to systems with a continuous eigenvalue spectrum in 1932 [33]. The history of these developments is fraught with intrigue, as discussed by Moore [45]; a comprehensive survey of the operator-theoretic developments in ergodic theory can be found in [16].

The Koopman operator $\mathcal{K}$ can be decomposed into sub-operators $\{\mathcal{K}_i\}_{i=1}^N$. A natural way to take advantage of this structure in solving (1.1) is by employing product formulas. The history of product formulas is complicated by gaps between theory and practice. Lie introduced (in 1875) the first operator splitting scheme recorded in history [38]. Motivated by the accurate solution of hyperbolic problems, Strang introduced a second order variant of the Lie scheme, based on a symmetrization principle [56]. The convergence of special algorithms for ordinary differential equations of course goes back to Euler and Picard. The same ideas prove the convergence of general algorithms for ordinary differential equations, as is given in numerical analysis.

Over the past two decades, Mezić and colleagues have extended Koopman theory from Hamiltonian systems with measure-preserving dynamics to encompass dissipative and non-smooth dynamics [42, 40, 41]. Additionally, Rowley et al [53] rigorously linked the Koopman mode decomposition, introduced by Mezić in 2005 [40], with the dynamic mode decomposition (DMD) algorithm, developed by Schmid in the fluid mechanics community [54, 55]. Recently, Koopman analysis has gained renewed attention, driven by the pioneering work of Mezić and collaborators [42, 40, 9, 41] and its significant connections to data-driven modeling techniques [55, 53, 37, 36]. This serendipitous connection not only provided a theoretical foundation for applying DMD to nonlinear systems but also paved the way for a powerful data-driven method to approximate the Koopman operator.

In the literature, three primary approaches have been proposed for approximating the Koopman semigroup: operator splitting schemes for approximating the Lie-Koopman semigroup [23, 10, 6, 27, 26, 11, 38, 29], spectral decomposition methods [41, 40, 16, 43, 44, 57], and data-driven approaches [55, 54, 60, 49, 51, 50, 39, 22].

This work investigates operator splitting schemes to approximate the Lie-Koopman generators of linear semigroups induced by non-linear flows. Our four main advances are as follows:

1. *Convergence and error bounds.* We analyze Lie-Trotter, Strang, and higher-order exponential splittings in strongly continuous and bicontinuous settings, and derive error bounds (Proposition 4.3, Theorems 4.5 and 4.8).
2. *Bi-continuous Chernoff extension.* We extend Chernoff's product formula to bicontinuous semigroups on bounded continuous functions arising from nonlinear flows, proving well-posedness and contraction of the splitting operators (Theorem 4.1).
3. *Explicit splitting algorithms.* In Section 4.4, we give coordinate-wise routines, freezing

variables and solving one-dimensional ODEs for each scheme, thus making high-order methods directly implementable with reduced effort.

4. *Numerical validation.* Section 5 benchmarks our methods on Lotka-Volterra, Van der Pol, and Lorenz systems, quantifying how RMSE scales with iteration count and splitting order.

2. Strongly continuous and bi-continuous semigroups. Let X be a Banach space over the complex numbers and $\mathcal{L}(X)$ be the set of bounded linear operators from X into X. A family $\{T(t), t \geq 0\} \subseteq \mathcal{L}(X)$ is called a *strongly continuous semigroup* if $T(0) = I$, if $T(t+r) = T(t)T(r)$ for all $t, r \geq 0$, and if for each $x \in X$ the map $t \to T(t)x$ is continuous on $[0, \infty)$. If $\{T(t), t \geq 0\} \subset \mathcal{L}(X)$ is a semigroup of linear operators, then the linear operator $\mathcal{A}$ defined by

$$D(\mathcal{A}) = \{x \in X : \lim_{t \to 0^+} \frac{T(t)x - x}{t} := y \text{ exists in } X\}, \ \mathcal{A}x := y \text{ for } x \in D(\mathcal{A})$$

is called the generator of the semigroup $\{T(t), t \geq 0\}$.

If the semigroup is strongly continuous, then the domain $D(\mathcal{A})$ is dense in X, $\mathcal{A}$ is a closed linear operator, and there exists $w \in \mathbb{R}$ such that $\lambda I - \mathcal{A}$ is invertible for all $\lambda \in \mathbb{C}$ with $Re(\lambda) > w$ (see [17]). Also, it is well known that all strongly continuous semigroups are *exponentially bounded*; i.e., if the three defining properties above hold, then there exist $M \geq 1$ and $\omega \in \mathbb{R}$ such that $\|T(t)\| \leq Me^{\omega t}$ for all $t \geq 0$, (see, e.g [17], page 39).

Example 2.1. *Let $\Omega = [0, \infty)$ and let $\sigma(t, x) = t + x$ denote the unique solution of $x'(t) = 1$ with initial condition $x(0) = x \in \Omega$. The induced Koopman-Lie semigroup is given by*

$$t \to T(t)g(x) = g(\sigma(t, x)) = g(t + x). \tag{2.1}$$

This defines a semigroup on $\mathcal{F} = \mathcal{F}(\Omega, \mathbb{C})$ and on all $T(t)$-invariant function spaces $\mathcal{M} \subset \mathcal{F}$. However, while the algebraic semigroup properties $T(0) = I$, and $T(t + r) = T(t)T(r)$ for all $t, r \geq 0$ hold on all $T(t)$-invariant $\mathcal{M} \subset \mathcal{F}$, the regularity property (3) depends heavily on $\mathcal{M}$. For example:

- *If $\mathcal{M} := C_0([0, \infty), \mathbb{C}) = \{g \in C_b([0, \infty), \mathbb{C}) : \lim_{x \to \infty} g(x) = 0\}$, then it can be easily seen that the semigroup (2.1) is strongly continuous since g vanishes at infinity and is uniformly continuous on compact intervals.*
- *If $\mathcal{M} := C_b([0, \infty), \mathbb{C})$, then the shift semigroup (2.1) is not strongly continuous. This can be seen by taking $g(x) = e^{ix^2}$. Then, $\|T(t + r)g - T(t)g\| = 2$ for all $t, r \geq 0$. So, $t \to T(t)g$ is nowhere continuous and, therefore, not measurable on $[0, \infty)$ since it is not almost separably valued (see, for example Pettis' Theorem in [1]).*

The shift semigroup (2.1) on $\mathcal{M} := C_b([0, \infty), \mathbb{C})$ is an example of a semigroup that is not strongly continuous but "*bi-continuous*". The bi-continuous semigroup framework, introduced by F. Kühnemund in her dissertation [35] at the University of Tübingen, provides an efficient approach to the work of Dorroh, Lovelady, Neuberger, and Sentilles, see [35], [18], and [19]. One of the key features of the bi-continuous semigroup framework is that many important results from the theory of strongly continuous semigroups can be lifted to bi-continuous semigroups.

The shift semigroup (2.1) on $\mathcal{M} := C_b([0,\infty),\mathbb{C})$ is bi-continuous in the following sense: for each $t \geq 0$, $T(t)$ is a continuous (bounded) linear operator from the Banach space $\mathcal{M}$ into itself with respect to norm topology on $\mathcal{M}$, while for each $f \in \mathcal{M}$ the map $t \to T(t)f$ from $[0,\infty) \to C_b([0,\infty),\mathbb{C})$ is continuous with respect to the compact-open topology, or equivalently, the topology of uniform convergence on compact sets. This leads to the concept of bi-admissible Banach spaces $(\mathcal{M}, ||\cdot||, \tau)$.

Definition 2.2. *Let $(X, \|\cdot\|)$ be a Banach space, and let τ be the topology generated by a family of seminorms $\{p_\alpha\}_{\alpha\in I}$ on X. Then $X = (X, \|\cdot\|, \tau)$ is a bi-admissible Banach space if p_α satisfies the following conditions:*

- $\|x\| = \sup_{\alpha\in I} p_\alpha(x)$ *for all* $x \in X$.
- *Every norm-bounded, p-Cauchy sequence is p-convergent in X.*
- $x = 0$ *if and only if* $p_\alpha(x) = 0$ *for all* $\alpha \in I$ *(separating).*
- *The space $(X,\tau)^*$ is norming for $(X, ||\cdot||)$; i.e., $||x|| = \sup\{|\phi(x)|\}$, where the supremum is taken over all $\phi \in (X,\tau)^* \subset (X, \|\cdot\|)^*$ with $\|\phi\| \leq 1$.*

Definition 2.3. *Let $(X, \|\cdot\|, \tau)$ be a bi-admissible Banach space. An operator family $\{T(t) : t \geq 0\} \subseteq \mathcal{L}(X)$ is a bi-continuous semigroup with respect to τ and of type ω if the following conditions hold:*

- $T(0) = I$ *and* $T(t+s) = T(t)T(s)$ *for all* $s, t \geq 0$.
- *The operators are exponentially bounded, i.e.; $\|T(t)\| \leq Me^{\omega t}$ for all $t \geq 0$ and some*

  constants $M \geq 1$ and $\omega \in \mathbb{R}$.
- *The map $t \to T(t)f$ $(t \geq 0)$ is strongly τ-continuous for each $f \in X$.*
- *$T(t)$ is locally bi-equicontinuous, where for every τ-convergent null sequence $f_n \subset X$,*

  $\tau\text{-}\lim_{n\to\infty} T(t)f_n = 0$ *uniformly for t in compact intervals of $\mathbb{R}_+$.*

As observed by Kühnemund in [35], it is one of the great advantages of the framework of bi-continuous semigroups, that many (most) of the central results of the theory of strongly continuous semigroups that are based on Laplace transform methods (see [2]) can be lifted to the bi-continuous case. To state the main properties of bi-continuous semigroups and their generators, the following definition is needed.

Definition 2.4. *Let $(X, \|\cdot\|, \tau)$ be a bi-admissible Banach space.*

- *A subset $D \subset X$ is called bi-dense if for every $g \in X$ there exists a $\|\cdot\|$-bounded sequence $g_n \in D$ which is τ−convergent to g.*
- *An operator $(\mathcal{K}, D(\mathcal{K}))$ is called bi-closed, if for all sequences $g_n \in D(\mathcal{K})$ that satisfy $\sup_{n\in\mathbb{N}}\{\|g_n\|, \|\mathcal{K}g_n\|\} < \infty$, $\tau - \lim g_n = g$, and $\tau - \lim \mathcal{K}g_n = f$, we have $g \in D(\mathcal{K})$ and $\mathcal{K}g = f$.*
- *The generator $(\mathcal{K}, D(\mathcal{K}))$ of a bi-continuous semigroup $T(t)$ on X is given by*

$$\mathcal{K}g := \tau - \lim_{t\to 0^+} \frac{T(t)g - g}{t}$$

for all $g \in D(\mathcal{K})$, where $D(\mathcal{K})$ denotes the set of all $g \in X$ such that τ-$\lim_{t\to 0^+} \frac{T(t)g-g}{t}$ exists and $\sup_{0<t\leq 1} \{\frac{\|T(t)g-g\|}{t}\}$ is finite.

3. Flows and Koopman semigroups. In this section, we review key definitions and properties of flows, introduce the Lie–Koopman generator, and present the Dorroh–Neuberger Theorem, which characterizes Koopman generators of continuous flows on Polish spaces [14].

Definition 3.1. *Let Ω be a set (called the* state space*). A function*

$$\sigma : [0,\infty) \times \Omega \to \Omega, \quad (t,x) \mapsto \sigma(t,x),$$

is called an autonomous, Ω-invariant flow map *if the following conditions hold:*
- *$\sigma(0,x) = x$ for all $x \in \Omega$;*
- *$\sigma(t,\sigma(r,x)) = \sigma(t+r,x)$ for all $x \in \Omega$ and all $t,r \geq 0$ with $t+r < \infty$;*
- *For every $x \in \Omega$, the trajectory $\sigma(t,x)$ remains in Ω for all $t \geq 0$.*

Then, the collection $\Sigma = \{\sigma(\cdot,x) : x \in \Omega\}$ is called an autonomous flow in Ω.

Definition 3.2. *Let $\Omega \subseteq \mathbb{R}^N$ be locally compact. A flow $\sigma : [0,\infty)\times\Omega \to \Omega$ is said to be jointly continuous if*
- *$t \to \sigma(t,x)$ is continuous for $t \in [0,\infty)$ for all $x \in \Omega$, and*
- *$x \to \sigma(t,x)$ is continuous on Ω for all $t \geq 0$. That is, if $x \in \Omega$, and $x_n \to x$, then $\sigma(t,x_n) \to \sigma(t,x)$.*

Definition 3.3. *Let $\Omega \subset \mathbb{R}^n$ be a space state, assume $F : \mathbb{R}^n \to \mathbb{R}^n$ where $x \in \Omega$, and let $t \to x(t) \in \mathbb{R}^n$ be a differentiable function for $t \in [0,\infty)$ that satisfies*

$$x'(t) = F(x(t)), \quad x(0) = x_0 = x \tag{3.1}$$

for all $t \in [0,\infty)$. Then $x(\cdot)$ is called a classical solution.

Proposition 3.4. *Assume that for all $x \in \Omega$, (3.1) has a unique classical solution $t \to x(t)$ for $0 \leq t < \infty$. If Ω is $[0,\infty)$-invariant, then*

$$t \to \sigma(t,x) := x(t) \quad (t \in [0,\infty))$$

defines an autonomous flow in Ω.

Proof. Let $t \to x(t) = \sigma(t,x)$ be the unique solution of (3.1) for $0 \leq t < \infty$. Assume that $0 \leq t, r, t+r < \infty$ and define

$$w(t) := x(t+r) = \sigma(t+r,x) \quad \text{for} \quad 0 \leq t+r < \infty.$$

Then $w(0) = x(r) = \sigma(r,x)$ and $w'(t) = x'(t+r) = F(x(t+r)) = F(w(t))$. By uniqueness,

$$\sigma(t+r,x) = w(t) = \sigma(t,\sigma(r,x)).$$

■

We now introduce the Lie–Koopman semigroup and explore its connection to the dynamics of the underlying flow. Let Ω be a set and $\mathcal{F}(\Omega,\mathbb{C})$ the vector space of all functions from Ω

into $\mathbb{C}$. The goal of “Koopmanism” is to show that for every autonomous, Ω-invariant flow Σ and appropriately chosen observation $g : \Omega \to \mathbb{C}$, there exists a linear Koopman operator $\mathcal{K}$ that “generates” the observations $t \to g(\sigma(t, x))$. The infinitesimal generator

$$\mathcal{K}g : x \to \lim_{t\to 0^+} \frac{T(t)g(x) - g(x)}{t} = \lim_{t\to 0^+} \frac{g(\sigma(t, x)) - g(x)}{t} \tag{3.2}$$

is always a well-defined linear operator with domain

$$D(\mathcal{K}) := \{g \in \mathcal{F}(\Omega, \mathbb{C}) : \text{limit in (3.2) exists for all } x \in \Omega\}$$

and range in $\mathcal{F}(\Omega, \mathbb{C})$. If Ω is a topological vector space, then $\mathcal{K}$ is given by

$$\mathcal{K}g(x) = T'(0)g(x) = g'(x) \cdot \sigma'(0, x), \tag{3.3}$$

and the Koopman semigroup associated to $\mathcal{K}$ is

$$T(t)g(x) = e^{t\mathcal{K}}g(x) = g(\sigma(t, x))$$

for all $x \in \Omega$ and $0 \leq t < \infty$. As seen above in Example 2.1, the Koopman semigroup $T(t)g(x) := g(\sigma(t, x))$ induced by a jointly continuous and global flow $\sigma : \mathbb{R}_+ \times \Omega$ in a Polish Space Ω may not always be strongly continuous for $g \in \mathbb{C}_b(\Omega)$ with respect to the sup-norm. However, in joint work done by J.R. Dorroh and J.W. Neuberger between 1990 and 1996, Koopman generators $(\mathcal{K}, D(\mathcal{K}))$ of jointly continuous and global flows on Ω were fully characterized, where the graph (g, f) consists of $g, f \in \mathbb{C}_b(\Omega)$ for which

$$\mathcal{K}g = f(x) = \lim_{t\to 0^+} \frac{g(\sigma(t, x)) - g(x)}{t} \text{ for all } x \in \Omega.$$

In the language of bi-continuous semigroups, the main result of the joint work of Dorroh and Neuberger [13, 15] concerning jointly continuous, global flows can be restated as follows.

Theorem 3.5. *Let Ω be a complete, separable, metric space (Polish space), and let $(\mathcal{K}, D(\mathcal{K}))$ be a linear operator on $C_b(\Omega)$. The following are equivalent:*

- *$(\mathcal{K}, D(\mathcal{K}))$ is the Koopman generator of a jointly continuous, global flow in Ω.*
- *$(\mathcal{K}, D(\mathcal{K}))$ is a derivation (i.e., $\mathcal{K}(fg) = (\mathcal{K}f)g + f(\mathcal{K}g)$ for all $f, g \in D(\mathcal{K})$ and generates a bi-continuous semigroup with respect to τ induced by a jointly continuous flow.*

In particular, Koopman semigroups induced by jointly continuous, global flows in a Polish space Ω are bi-continuous contractions in $(C_b(\Omega), \|\cdot\|_\infty, \tau)$.

4. Splitting Methods. To solve differential equations numerically, one can often use operator splitting methods, which simplify the numerical treatment of certain differential equations. The concept involves decomposing the original equation into sub-problems, with each sub-problem treated independently. By applying effective numerical methods to each sub-problem, or by solving each sub-problem explicitly, one can then achieve good approximations of the solutions to the original problems by appropriately reassembling the solutions of the sub-problems.

In practice, let $F:\mathbb{R}^N\to\mathbb{R}^N$ be given by $F=(F_1,...,F_N)$ where $F_i:\mathbb{R}^N\to\mathbb{R}$ and assume that $x'(t)=F(x(t))$, $x(0)=x\in\Omega\subset\mathbb{R}^N$ has a unique classical solution $\sigma(t,x):=x(t)$ for all $x\in\Omega$ and $0\le t<\infty$. Then it is easy to see that $t\to\sigma(t,x):=x(t)$ defines an autonomous flow and that the corresponding Koopman-Lie generator of the semigroup flow $T(t)g(x):=g(\sigma(t,x))$ is given by

$$\begin{aligned}\mathcal{K}g(x) :=& \lim_{t\to 0}\frac{g(\sigma(t,x))-g(x)}{t}=\frac{dg(\sigma(t,x))}{dt}\bigg|_{t=0}\\ =&g'(\sigma(t,x))\cdot\sigma'(t,x)\bigg|_{t=0}=g'(x(0))\cdot F(x(0))=g'(x)\cdot F(x)\\ =&\sum_{i=1}^N\frac{\partial g}{\partial x_i}(x)\cdot F_i(x)=\sum_{i=1}^N\mathcal{K}_i g(x),\end{aligned}\tag{4.1}$$

where $\mathcal{K}_i g(x)=\frac{\partial g}{\partial x_i}(x)\cdot F_i(x)$ generates the semigroup

$$e^{t\mathcal{K}_i}g(x)=g(x_1,...,x_{i-1},\sigma_i(t,x_i),x_{i+1},...,x_N),\tag{4.2}$$

and where $\sigma_i(t,x_i)$ solves the one-dimensional, separable equation

$$u'(t)=F_i(x_1,x_2,...,x_{i-1},u(t),x_{i+1},...,x_N)\text{ with }u(0)=x_i.\tag{4.3}$$

For flows $t\to\sigma(t,x)$ induced by solutions of ordinary differential equation $x'(t)=F(x(t))$, $x(0)=x\in\Omega$, the induced linear semigroup flow $t\to T(t)g(x)=g(\sigma(t,x))$ has a Koopman-Lie generator $\mathcal{K}$ that splits into a sum of one-dimensional Koopman-Lie generators $\mathcal{K}_i$, i.e.,

$$\mathcal{K}=\mathcal{K}_1+\mathcal{K}_2+...+\mathcal{K}_N.$$

Since computing

$$T(t)g(x)=e^{t\mathcal{K}}g(x)=e^{t(\mathcal{K}_1+\mathcal{K}_2+...+\mathcal{K}_N)}g(x),$$

is challenging and computationally expensive, by splitting the problem into one-dimensional subproblems $T_i(t)g(x)=e^{t\mathcal{K}_i}g(x)$, where each subproblem can be computed explicitly via separation of variables for all $1\le i\le N$, the computation becomes more manageable. As we shall see in the following section on "Chernoff's Product Formula", one can approximate

$$e^{t\mathcal{K}}g(x)=e^{t(\mathcal{K}_1+\cdots\mathcal{K}_N)}g(x)=g(\sigma(t,x))$$

in terms of operators like

$$V(t)g(x):=e^{t\mathcal{K}_1}\circ\cdots\circ e^{t\mathcal{K}_N}g(x)$$

for which $V(0)=I$ and $V'(0)=\mathcal{K}$.

4.1. Exponential Product Formulas. A key result of semigroup theory includes [17], [46], [24], [52], and most importantly for our purposes the work of Franziska Kühnemund [35] in which she extends the result to the bi-continuous case.

For Chernoff's product formula to hold in a Banach space X, let

$$V(\cdot):[0,\infty)\to\mathcal{L}(X)$$

satisfy $V(0) = I$, $\|V(t)^m\| \leq M$ for all $t \geq 0$, $m \in \mathbb{N}$, and some $M \geq 1$ and assume that

$$\mathcal{K}x := \lim_{h \to 0^+} \frac{V(h)x - x}{h}$$

exists for all $x \in D \subset X$, where D and $(\lambda_0 - \mathcal{K})D$ are dense subspaces in X for some $\lambda_0 > 0$. Then the closure $\bar{\mathcal{K}}$ of $\mathcal{K}$ generates a strongly continuous semigroup $(T(t))_{t \geq 0}$ with $\|T(t)\| \leq M(t \geq 0)$ which is given by

$$T(t)x = \lim_{n \to \infty} V(\frac{t}{n})^n x. \tag{4.4}$$

for all $x \in X$ and where the limit exists uniformly for t in compact intervals.

In order to estimate the speed of convergence, one can employ the non-commutative binomial theorem as follows. Let $h = \frac{t}{n}$. Then

$$\begin{aligned}
\|V(h)^n - T(t)\| = \|V(h)^n - T(h)^n\| &\leq \|\sum_{k=0}^{n-1} V(h)^{n-1-k} \Big[V(h) - T(h)\Big] T(h)^k\| \\
&\leq \sum_{k=0}^{n-1} \|V(h)^{n-1-k}\| \| \Big[V(h) - T(h)\Big] T(h)^k\| \\
&\leq M \sum_{k=0}^{n-1} \| \Big[V(h) - T(h)\Big] T(kh)\| \leq nM^2 \|V(h) - T(h)\|.
\end{aligned}$$

The inequality above indicates that the error estimates for $\|(V(h)^n x - T(t)x\|$ can be derived from an estimate of $\|V(h) - T(h)\|$ for small values of h. To do so, one considers approximations $V(t)$ that are *"of order p"*; that is $V(t)$ for which, in the case of matrices, the first p Taylor coefficients coincide with the first p Taylor coefficients of

$$T(t)x = e^{t\mathcal{K}}x = x + t\mathcal{K}x + \frac{t^2}{2!}\mathcal{K}^2 x + \cdots + \frac{t^p}{p!}\mathcal{K}^p x + \cdots .$$

Then, formally, for small values of h, one would then expect to obtain an estimate like

$$\begin{aligned}
&\|V(h)x - T(h)x\| \\
&\qquad \leq \| \frac{h^{p+1}}{(p+1)!}(V(0)^{p+1}x - \mathcal{K}^{p+1}x) + \frac{h^{p+2}}{(p+2)!}(V(0)^{p+2}x - \mathcal{K}^{p+2}x) + \cdots \| \\
&\qquad \leq \frac{h^{p+1}}{(p+1)!}\tilde{M}_x
\end{aligned} \tag{4.5}$$

for some $\tilde{M}_x \geq 0$. Together with estimate (4.1), and setting $h = \frac{t}{n}$, we would then have

$$\|(V(\frac{t}{n})^n x - T(t)x\| \leq \frac{1}{n^p} \frac{t^{p+1}}{(p+1)!} M^2 \tilde{M}_x. \tag{4.6}$$

In 2009, E. Hansen and A. Ostermann showed in [26] and [27] that the estimates (4.5) and (4.6) hold for splitting methods of the form

$$V(t) := \prod_{j=1}^{s} e^{\alpha_{j,1}t\mathcal{K}_1} \cdots e^{\alpha_{j,N}t\mathcal{K}_N}, \tag{4.7}$$

where $T(t) = e^{t\mathcal{K}}$ and $\mathcal{K} = \mathcal{K}_1 + \ldots \mathcal{K}_N$, and where the real or complex coefficients α_j's and β_j's are chosen in such a way that the method $V(t)$ has algebraic order p. For more details, see Section 3.4. Many of the central results of the theory of strongly continuous semigroups, especially those based on Laplace transform methods, can be lifted to the bi-continuous case, [35]. One of the significant results is that Chernoff's product formula extends to bi-continuous semigroups.

Theorem 4.1. *(Chernoff's Bi-Continuous Product Formula) Let $(\mathcal{K}, D(\mathcal{K}))$ be a linear operator on a bi-admissible Banach space $(X, \|\cdot\|, \tau)$, where $D(\mathcal{K})$ and $(\lambda_0 I - \mathcal{K})D(\mathcal{K})$ are bi-dense in X for some $\lambda_0 > \omega \geq 0$. Moreover, let $V(t) \in \mathcal{L}(X)$ be such that $||V(t)^n|| \leq Me^{\omega nt}$ for all $n \in \mathbb{N}_0$ and $t \in [0, \delta)$. If*

$$V'(0+)g = \|\cdot\| - \lim_{t\to 0^+} \frac{V(t)g - g}{t} = \mathcal{K}g$$

for all $g \in D(\mathcal{K})$ and if $\{V(t)^m : t \geq 0\}$ is locally bi-equicontinuous uniformly for $m \in \mathbb{N}$, then the bi-closure of $(\mathcal{K}, D(\mathcal{K}))$ generates a bi-continuous semigroup $T(t)$ and

$$T(t)g = \tau - \lim_{n\to\infty} \left(V(\frac{t}{n})\right)^n g \tag{4.8}$$

for all $g \in X$ and $t \geq 0$ uniformly in t on compact intervals.

Proof. See [35]. ∎

If one applies (4.8 to bi-continuous Koopman-Lie semigroups on $C_b(\Omega)$, then one obtains that

$$T(t)g(\cdot) = g(\sigma(t,\cdot)) = \tau - \lim_{n\to\infty} \left(V(\frac{t}{n})\right)^n g(\cdot) = \tau - \lim_{n\to\infty} g(\sigma_n(t,\cdot)) \tag{4.9}$$

uniformly in compact time intervals for all $g \in C_b(\Omega)$. The following proposition, due to Arun Banjara [3], shows that (4.9) implies that, for all $x \in \Omega$,

$$\sigma(t,x) = \lim_{n\to\infty} \sigma_n(t,x). \tag{4.10}$$

Definition 4.2. *Let Ω be a metric space. Then, for $x_n, x \in \Omega$, we say that x_n is weak-$C_b(\Omega)$ convergent to x and write $x_n \xrightarrow{C_b(\Omega)} x$ if $g(x_n) \to g(x)$ for all $g \in C_b(\Omega)$.*

Proposition 4.3. *Let $\Omega \subset \mathbb{R}^N$. Then the following statements are equivalent.*

a) $x_n \to x$ as $n \to \infty$,
b) $g(x_n) \to g(x)$ as $n \to \infty$ for all $g \in C_b(\Omega, \mathbb{R})$.

Proof. See Appendix A. ■

Many approximation formulas can be derived from Chernoff's Product Formula. For example,

(1) $V(t) := e^{t\mathcal{K}_1}e^{t\mathcal{K}_2}$, where $e^{t\mathcal{K}_1}$ and $e^{t\mathcal{K}_2}$ are strongly continuous or bi-continuous contraction semigroups on a Banach space X with generators $(\mathcal{K}_1, D(\mathcal{K}_1))$ and $(\mathcal{K}_2, D(\mathcal{K}_2))$, respectively. Then $V(0) = I$ and $\|V(t)^m\| \leq 1$ for all $t \geq 0$, $m \in \mathbb{N}$ and

$$\begin{aligned} \mathcal{K}x &= \lim_{h\to 0^+} \frac{V(h)x - x}{h} = \lim_{h\to 0^+} \frac{T_1(h)T_2(h)x - x}{h} \\ &= \lim_{h\to 0^+} T_1(h)\frac{T_2(h)x - x}{h} + \lim_{h\to 0^+} \frac{T_1(h)x - x}{h} \\ &= \mathcal{K}_2 x + \mathcal{K}_1 x. \end{aligned} \tag{4.11}$$

So, consider $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2$ on $D := D(\mathcal{K}_1) \cap D(\mathcal{K}_2)$ and assume that D and $(\lambda_0 - \mathcal{K}_1 - \mathcal{K}_2)D$ are dense in X. Then, by Chernoff's theorem,

$$\mathcal{K} := \overline{\mathcal{K}_1 + \mathcal{K}_2}$$

generates a strongly continuous semigroup $(T(t))_{(t\geq 0)}$ given by the *Lie-Trotter product formula*

$$T(t)x = \lim_{n\to\infty} \left(e^{\frac{t}{n}\mathcal{K}_1} e^{\frac{t}{n}\mathcal{K}_2} \right)^n x \tag{4.12}$$

for all $x \in X$ and the limit is uniform for t in compact intervals. The Lie-Trotter product formula has approximation order 1; that is, in general there exists a constant $M_{g,t}$ such that

$$\|T(t)x - \left(V(\frac{t}{n}) \right)^n x\| \leq \frac{M_{x,t}}{n}.$$

(2) If $V(t) := e^{\frac{t}{2}\mathcal{K}_2}e^{t\mathcal{K}_1}e^{\frac{t}{2}\mathcal{K}_2}$. Then, by Chernoff's theorem,

$$\mathcal{K} := \overline{\mathcal{K}_1 + \mathcal{K}_2}$$

generates a strongly continuous semigroup $(T(t))_{(t\geq 0)}$ given by the *Strang product formula*

$$T(t)x = \lim_{n\to\infty} \left(e^{\frac{t}{2n}\mathcal{K}_2} e^{\frac{t}{n}\mathcal{K}_1} e^{\frac{t}{2n}\mathcal{K}_2} \right)^n x \tag{4.13}$$

for all $x \in X$ and the limit is uniform for t in compact intervals. In general, the Strang product formula has approximation order 2; that is, in general there exists a constant $M_{g,t}$ such that

$$\|T(t)x - \left(V(\frac{t}{n}) \right)^n x\| \leq \frac{M_{x,t}}{n^2}.$$

Remark 4.4. The Lie-Trotter and Strang product formulas can also be employed in cases where the Koopman-Lie generator $\mathcal{K}$ can be split into N simpler parts $\mathcal{K} = \mathcal{K}_1 + \cdots + \mathcal{K}_N$. Then we can rewrite the Lie-Trotter and Strang product formulas, as follows:

(3) If $V(t) := e^{t\mathcal{K}_1} e^{t\mathcal{K}_2} \cdots e^{t\mathcal{K}_N}$. Then, the higher dimensional Lie-Trotter product formula is given by

$$T(t)x = \lim_{n\to\infty} \left(e^{\frac{t}{n}\mathcal{K}_1} e^{\frac{t}{n}\mathcal{K}_2} \cdots e^{\frac{t}{n}\mathcal{K}_N} \right)^n x. \tag{4.14}$$

(4) If $V(t) := e^{\frac{t}{2}\mathcal{K}_N} \cdots e^{t\mathcal{K}_1} \cdots e^{\frac{t}{2}\mathcal{K}_N}$. Then, the higher dimensional Strang product formula is given by

$$T(t)x = \lim_{n\to\infty} \left(e^{\frac{t}{2n}\mathcal{K}_N} \cdots e^{\frac{t}{2n}\mathcal{K}_2} e^{\frac{t}{n}\mathcal{K}_1} e^{\frac{t}{2n}\mathcal{K}_2} \cdots e^{\frac{t}{2n}\mathcal{K}_N} \right)^n x. \tag{4.15}$$

4.2. Higher-order Exponential Splitting Schemes. In [26] and [27], E. Hansen and A. Ostermann consider exponential splitting schemes

$$V_p(t) := \prod_{j=1}^{s} e^{\alpha_j t\mathcal{K}_1} e^{\beta_j t\mathcal{K}_2}, \tag{4.16}$$

where the real or complex coefficients α_j's and β_j's are chosen in such a way that the method is algebraically of order p, meaning that whenever the operators $\mathcal{K}, \mathcal{K}_i$ are replaced by finite matrices $\mathcal{M}, \mathcal{M}_i$, we have

$$\|V(t) - e^{t\mathcal{M}}\| = O(t^{p+1}).$$

For example, to obtain a 3-stage splitting of the form (4.16), consider

$$\mathcal{K} = \alpha_1\mathcal{K}_1 + \beta_1\mathcal{K}_2 + \alpha_2\mathcal{K}_1 + \beta_2\mathcal{K}_2 + \alpha_3\mathcal{K}_1 + \beta_3\mathcal{K}_2$$

with $\alpha_1 + \alpha_2 + \alpha_3 = 1$, $\beta_1 + \beta_2 + \beta_3 = 1$ for which the associated product formula

$$V(t) = e^{\alpha_1 t\mathcal{K}_1} e^{\beta_1 t\mathcal{K}_2} e^{\alpha_2 t\mathcal{K}_1} e^{\beta_2 t\mathcal{K}_2} e^{\alpha_3 t\mathcal{K}_1} e^{\beta_3 t\mathcal{K}_2}$$

is algebraically of order $p = 3$. For such s-stage schemes, they provide a general error-estimate framework for the approximations of solutions of linear problems of the form

$$x'(t) = \mathcal{K}x(t) = (\mathcal{K}_1 + \mathcal{K}_2)x(t), \;\; x(0) = x \tag{4.17}$$

where $\mathcal{K}_1$, $\mathcal{K}_1$, and $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2$ are generators of strongly continuous contraction semigroups (or analytic contraction semigroups if the coefficients α_j's and β_j's are complex). Their analysis is based on the consideration of the operators E_{p+1} that can be obtained as the product of exactly $p+1$ factors chosen among $\mathcal{K}_1$ or $\mathcal{K}_2$.

Theorem 4.5. *[26], [27]. Let $\mathcal{K}_1$, $\mathcal{K}_2$, and $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2$ be generators of strongly continuous contraction semigroups on a Banach space X (or analytic contraction semigroups if the coefficients α_j's and β_j's are complex). Assume that there exists a subspace $U \subset D(\mathcal{K}^{p+1})$ such that all $E_{p+1}e^{t\mathcal{K}} : U \to X$ are well defined and all $E_{p+1}e^{t\mathcal{K}}u$ are uniformly bounded in $t \in [0,T]$ for any $u \in U$. Then, for all $u \in U$ and $T > 0$, there exists a constant $M_{u,T}$ such that*

$$\|V_p(\frac{t}{n})^n u - e^{t\mathcal{K}}u\| \leq M_{u,T}\frac{t^{p+1}}{n^p(p+1)!}, \quad 0 \leq t \leq T. \tag{4.18}$$

Outline of proof: The proof is based on estimate of the form (4.1); i.e,

$$\begin{aligned} \|V_p(\frac{t}{n})^n x - (e^{\frac{t\mathcal{K}}{n}})^n x\| &= \|\sum_{j=0}^{n-1} V_p(\frac{t}{n})^{n-j-1}(V_p(\frac{t}{n}) - e^{\frac{t\mathcal{K}}{n}})e^{j\frac{t\mathcal{K}}{n}}x\| \\ &\leq \sum_{j=0}^{n-1} \|(V_p(\frac{t}{n}) - e^{\frac{t\mathcal{K}}{n}})e^{j\frac{t\mathcal{K}}{n}}x\| \end{aligned} \tag{4.19}$$

and a sophisticated and elaborate estimate of the term $\|(V_p(\frac{t}{n}) - e^{\frac{t\mathcal{K}}{n}})e^{j\frac{t\mathcal{K}}{n}}x\|$.

Remark 4.6. Since the proof of Theorem 4.5 given in [26] is of an algebraic nature, it can be extended to bi-continuous contraction semigroups without changing any of arguments.

The coefficients α_i and β_i are chosen such that the first four terms of the Taylor expansions coincide, in order to obtain a classical method of order 3. By comparing these coefficients, one can derive the following proposition.

Proposition 4.7. *Let $\alpha = \frac{1}{2} + \frac{i\sqrt{3}}{6}$ and*

$$V_3(t) = e^{\alpha\frac{t}{2}\mathcal{K}_2}e^{\alpha t\mathcal{K}_1}e^{\frac{t}{2}\mathcal{K}_2}e^{\bar{\alpha}t\mathcal{K}_1}e^{\bar{\alpha}\frac{t}{2}\mathcal{K}_2}. \tag{4.20}$$

Then the formula of the complex product $V_3(t)$ is algebraically of order $p = 3$.

Proof. See [27] and [25]. ∎

Deriving higher-order methods by comparing coefficients becomes increasingly challenging as the number of coefficients grows rapidly. To overcome these algebraic complexities, the following statements explore how higher-order splitting schemes can be constructed by composing lower-order schemes. Specifically, they provide higher-order product formulas for splittings of the form $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2$ and $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2 + \cdots + \mathcal{K}_N$, developed using composition methods by F. Castella, P. Chartier, S. Descombes, and G. Vilmart, as well as E. Hansen and A. Ostermann in 2009 (see [27] and [52]). We follow the exposition given in [27].

Theorem 4.8. *Let $U_{[0]}(t) := V_2(t) = e^{\frac{t}{2}\mathcal{K}_2}e^{t\mathcal{K}_1}e^{\frac{t}{2}\mathcal{K}_2}$. For $1 \leq k \leq 4$ define*

$$U_{[k]}(t) := U_{[k-1]}(\bar{a}_k t)U_{[k-1]}(a_k t) \quad \text{with } a_k := \frac{1}{2} + i\frac{\sin(\pi/(k+2))}{2 + 2\cos(\pi/(k+2))}. \tag{4.21}$$

Then the splitting schemes $U_{[k]}(t)$ are of order $k+2$ and have $2^{k+1}+1$ exponential terms. In particular,

$$U_{[1]}(t) = e^{\bar{a}\frac{t}{2}\mathcal{K}_2} e^{\bar{a}t\mathcal{K}_1} e^{\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{a\frac{t}{2}\mathcal{K}_2} \tag{4.22}$$

has 5 terms, and is of order 3, where $a = \frac{1}{2} + i\frac{\sqrt{3}}{6} = 0.5 + 0.28875i$.

$$U_{[2]}(t) = e^{\bar{a}\frac{t}{2}\mathcal{K}_2} e^{\bar{a}t\mathcal{K}_1} e^{(\bar{a}+\bar{b})\frac{t}{2}\mathcal{K}_2} e^{\bar{b}t\mathcal{K}_1} e^{\Re(b)t\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{(a+b)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{a\frac{t}{2}\mathcal{K}_2} \tag{4.23}$$

has 9 terms, and is of order 4, where

$$\begin{aligned} a &= \frac{1}{12}(3+\sqrt{3}-\sqrt{6}) + i\frac{1}{12}(3-3\sqrt{2}-\sqrt{3}) = 0.190213 + 0.247891i, \\ b &= \frac{1}{12}(3-\sqrt{3}+\sqrt{6}) - i\frac{1}{12}(3-3\sqrt{2}+\sqrt{3}) = 0.309787 - 0.0407842i. \end{aligned}$$

$$\begin{aligned} U_{[3]}(t) = {} & e^{\bar{a}\frac{t}{2}\mathcal{K}_2} e^{\bar{a}t\mathcal{K}_1} e^{(\bar{a}+\bar{b})\frac{t}{2}\mathcal{K}_2} e^{\bar{b}t\mathcal{K}_1} e^{(\bar{b}+\bar{c})\frac{t}{2}\mathcal{K}_2} e^{\bar{c}t\mathcal{K}_1} e^{(\bar{c}+\bar{d})\frac{t}{2}\mathcal{K}_2} e^{\bar{d}t\mathcal{K}_1} e^{\Re(d)t\mathcal{K}_2} e^{dt\mathcal{K}_1} e^{(c+d)\frac{t}{2}\mathcal{K}_2} \\ & e^{ct\mathcal{K}_1} e^{(b+c)\frac{t}{2}\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{(b+a)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{a\frac{t}{2}\mathcal{K}_2} \end{aligned}$$

has 17 terms, and is of order 5, where

$$\begin{aligned} a &= 0.054834 + 0.154848i, & c &= 0.148267 + 0.07072i, \\ b &= 0.161519 + 0.0299358i, & d &= 0.135379 - 0.0930434i. \end{aligned}$$

$$\begin{aligned} U_{[4]}(t) = {} & e^{\bar{a}\frac{t}{2}\mathcal{K}_2} e^{\bar{a}t\mathcal{K}_1} e^{(\bar{a}+\bar{b})\frac{t}{2}\mathcal{K}_2} e^{\bar{b}t\mathcal{K}_1} e^{(\bar{b}+\bar{c})\frac{t}{2}\mathcal{K}_2} e^{\bar{c}t\mathcal{K}_1} e^{(\bar{c}+\bar{d})\frac{t}{2}\mathcal{K}_2} e^{\bar{d}t\mathcal{K}_1} e^{\bar{e}\frac{t}{2}\mathcal{K}_2} e^{\bar{e}t\mathcal{K}_1} e^{(\bar{e}+\bar{f})\frac{t}{2}\mathcal{K}_2} \\ & e^{\bar{f}t\mathcal{K}_1} e^{(\bar{f}+\bar{g})\frac{t}{2}\mathcal{K}_2} e^{\bar{g}t\mathcal{K}_1} e^{(\bar{g}+\bar{h})\frac{t}{2}\mathcal{K}_2} e^{\bar{h}t\mathcal{K}_1} e^{\Re(h)t\mathcal{K}_2} e^{ht\mathcal{K}_1} e^{(g+h)\frac{t}{2}\mathcal{K}_2} e^{gt\mathcal{K}_1} e^{(f+g)\frac{t}{2}\mathcal{K}_2} e^{ft\mathcal{K}_1} \\ & e^{(e+f)\frac{t}{2}\mathcal{K}_2} e^{et\mathcal{K}_1} e^{(d+e)\frac{t}{2}\mathcal{K}_2} e^{dt\mathcal{K}_1} e^{(c+d)\frac{t}{2}\mathcal{K}_2} e^{ct\mathcal{K}_1} e^{(b+c)\frac{t}{2}\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{(b+a)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{a\frac{t}{2}\mathcal{K}_2} \end{aligned}$$

has 33 terms, and is of order 6, where

$$\begin{aligned} a &= 0.006672 + 0.084770i, & e &= 0.055224 + 0.064659i, \\ b &= 0.076749 + 0.036607i, & f &= 0.083608 - 0.015496i, \\ c &= 0.064659 + 0.055224i, & g &= 0.084770 + 0.006672i, \\ d &= 0.080155 - 0.028384i, & h &= 0.048163 - 0.070077i. \end{aligned}$$

Proof. The statement (4.21) is shown in [27], Theorem 2.2. ■

The remaining theorems follow by analogous arguments, employing techniques similar to those above, and are reformulations of Theorems 2.3 and 2.4 in [27].

Theorem 4.9. *Let* $W_{[0]}(t) := V_2(t) = e^{\frac{t}{2}\mathcal{K}_2} e^{t\mathcal{K}_1} e^{\frac{t}{2}\mathcal{K}_2}$. *For* $1 \le k \le 3$ *define*

$$W_{[k]}(t) := W_{[k-1]}(a_k t) W_{[k-1]}((1-2a_k)t) W_{[k-1]}(a_k t) \tag{4.24}$$

with

$$a_k = \frac{e^{\pi i/(2k+1)}}{2^{1/(2k+1)} + e^{\pi i/(2k+1)}}.$$

Then the splitting schemes $W_{[k]}(t)$ *are of order* $2k+2$ *and have* $2(3^k)+1$ *exponential terms. In particular,*

$$W_{[1]}(t) = e^{a\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(1-a)\frac{t}{2}\mathcal{K}_2} e^{(1-2a)t\mathcal{K}_1} e^{(1-a)t\mathcal{K}_2} e^{at\mathcal{K}_1} e^{a\frac{t}{2}\mathcal{K}_2} \tag{4.25}$$

has 7 terms and is of order 4, where $a = 0.324396 + 0.134586i$.

$$\begin{aligned} W_{[2]}(t) = {} & e^{a\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+b)\frac{t}{2}\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{(a+b)t\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+c)\frac{t}{2}\mathcal{K}_2} e^{ct\mathcal{K}_1} e^{(c+d)\frac{t}{2}\mathcal{K}_2} e^{dt\mathcal{K}_1} e^{(c+d)\frac{t}{2}\mathcal{K}_2} \\ & e^{ct\mathcal{K}_1} e^{(a+c)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+b)t\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{(a+b)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{a\frac{t}{2}\mathcal{K}_2} \end{aligned}$$

has 19 terms, and is of order 6, where

$$\begin{aligned} a &= 0.095099 + 0.067864i, & c &= 0.134198 - 0.001142i, \\ b &= 0.133957 - 0.061013i, & d &= 1 - 2a. \end{aligned}$$

$$\begin{aligned} W_{[3]}(t) = {} & e^{a\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+b)\frac{t}{2}\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{(a+b)t\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+c)\frac{t}{2}\mathcal{K}_2} e^{ct\mathcal{K}_1} e^{(c+d)\frac{t}{2}\mathcal{K}_2} e^{dt\mathcal{K}_1} e^{(c+d)\frac{t}{2}\mathcal{K}_2} \\ & e^{ct\mathcal{K}_1} e^{(a+c)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+b)t\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{(a+b)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+e))\frac{t}{2}\mathcal{K}_2} e^{et\mathcal{K}_1} e^{(e+f)\frac{t}{2}\mathcal{K}_2} e^{ft\mathcal{K}_1} \\ & e^{(e+f)t\mathcal{K}_2} e^{et\mathcal{K}_1} e^{(e+g)\frac{t}{2}\mathcal{K}_2} e^{gt\mathcal{K}_1} e^{(g+h))\frac{t}{2}\mathcal{K}_2} e^{ht\mathcal{K}_1} e^{(g+h)\frac{t}{2}\mathcal{K}_2} e^{gt\mathcal{K}_1} e^{(g+e)t\mathcal{K}_2} e^{et\mathcal{K}_1} e^{(e+f)\frac{t}{2}\mathcal{K}_2} \\ & e^{ft\mathcal{K}_1} e^{(e+f))\frac{t}{2}\mathcal{K}_2} e^{et\mathcal{K}_1} e^{(a+e)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+b)\frac{t}{2}\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{(a+b)t\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+c)\frac{t}{2}\mathcal{K}_2} e^{ct\mathcal{K}_1} \\ & e^{(c+d)\frac{t}{2}\mathcal{K}_2} e^{dt\mathcal{K}_1} e^{(c+d)\frac{t}{2}\mathcal{K}_2} e^{ct\mathcal{K}_1} e^{(a+c)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+b)t\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{(a+b)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{a\frac{t}{2}\mathcal{K}_2} \end{aligned}$$

has 55 terms, and is of order 8, where

$$\begin{aligned} a &= 0.027429 + 0.027049i, & e &= 0.040242 + 0.013767i, \\ b &= 0.046792 - 0.012888i, & f &= 0.0403725 - 0.035236i, \\ c &= 0.043753 + 0.006617i, & g &= 0.046693 - 0.014377i, \\ d &= 0.034783 - 0.043571i, & h &= 0.0137277 - 0.060005i. \end{aligned}$$

Proof. The proof of statement (4.24) is analogous to the proof of Theorem 2.3 in [27]. ∎

Theorem 4.10. *Let* $Z_{[0]}(t) := V_2(t) = e^{\frac{t}{2}\mathcal{K}_2} e^{t\mathcal{K}_1} e^{\frac{t}{2}\mathcal{K}_2}$. *For* $1 \le k \le 6$ *define*

$$Z_{[k]}(t) := Z_{[k-1]}(a_k t) Z_{[k-1]}(\bar{a}_k t) Z_{[k-1]}(\bar{a}_k t) Z_{[k-1]}(a_k t) \tag{4.26}$$

with

$$a_k := \frac{1}{4} + i\frac{\sin(\pi/(2k+1))}{4 + 4\cos(\pi/(2k+1))}.$$

Then the splitting schemes $Z_{[k]}(t)$ *are of order* $2k+2$ *and have* $2(4^k)+1$ *exponential terms. In particular,*

$$Z_{[1]}(t) = e^{a\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{\frac{t}{4}\mathcal{K}_2} e^{\bar{a}t\mathcal{K}_1} e^{\bar{a}t\mathcal{K}_2} e^{\bar{a}t\mathcal{K}_1} e^{\frac{t}{4}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{a\frac{t}{2}\mathcal{K}_2}$$

has 9 terms and is of order 4, where $a = 0.25 + 0.144338i$.

$$\begin{aligned} Z_{[2]}(t) = {} & e^{a\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+b)\frac{t}{2}\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{bt\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{(a+b)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+\bar{b})\frac{t}{2}\mathcal{K}_2} e^{\bar{b}t\mathcal{K}_1} e^{(\bar{a}+\bar{b})t\mathcal{K}_2} \\ & e^{\bar{a}t\mathcal{K}_1} e^{\bar{a}t\mathcal{K}_2} e^{\bar{a}t\mathcal{K}_1} e^{(\bar{a}+\bar{b})t\mathcal{K}_2} e^{\bar{b}t\mathcal{K}_1} e^{\bar{b}t\mathcal{K}_2} e^{\bar{b}t\mathcal{K}_1} e^{(\bar{a}+\bar{b})t\mathcal{K}_2} e^{\bar{a}t\mathcal{K}_1} e^{\bar{a}t\mathcal{K}_2} e^{\bar{a}t\mathcal{K}_1} e^{(\bar{a}+\bar{b})t\mathcal{K}_2} \\ & e^{\bar{b}t\mathcal{K}_1} e^{(a+\bar{b})t\mathcal{K}_2} e^{at\mathcal{K}_1} e^{(a+b)\frac{t}{2}\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{bt\mathcal{K}_2} e^{bt\mathcal{K}_1} e^{(a+b)\frac{t}{2}\mathcal{K}_2} e^{at\mathcal{K}_1} e^{a\frac{t}{2}\mathcal{K}_2} \end{aligned}$$

has 33 terms, and is of order 6, where

$$\begin{aligned} a &= 0.050776 + 0.056392i \\ b &= 0.074225 - 0.015777i \end{aligned}$$

Moreover, $Z_{[3]}$ *has 129 terms and is of order 8,* $Z_{[4]}$ *has 513 terms and is of order 10,* $Z_{[5]}$ *has 2049 terms and is of order 12, and* $Z_{[6]}$ *has 8193 terms and is of order 14.*

Proof. The proof of statement (4.26) is analogous to the proof of Theorem 2.4 in [27]. ■

4.3. Estimating the Number of Exponential Terms in Higher-Dimensional Problem. In this subsection, we present an algorithm to compute the number of exponential terms required for higher-dimensional splitting methods. We begin with the classical Lie–Trotter and Strang product formulas, which can be extended to N-dimensional systems. The Lie–Trotter splitting, of algebraic order $p = 1$, requires N exponential terms when $N > 1$. In contrast, the Strang splitting, of order $p = 2$, necessitates $2N - 1$ exponential terms for the same case. These constructions are illustrated with concrete examples.

To explore higher-order methods, we examine the structure of their exponential compositions. For instance, a third-order scheme in two dimensions takes the form:

$$V(t) = e^{b_1 t\mathcal{K}_2} e^{a_1 t\mathcal{K}_1} e^{b_2 t\mathcal{K}_2} e^{a_2 t\mathcal{K}_1} e^{b_3 t\mathcal{K}_2}, \quad \text{such that} \quad V'(0) = \mathcal{K}_1 + \mathcal{K}_2.$$

This structure includes five exponential terms and maintains consistency with the required generator.

To generalize the construction for higher dimensions, let A, B, C, D, E represent exponentials of $\mathcal{K}_1, \mathcal{K}_2, \ldots, \mathcal{K}_5$, respectively. We propose a recursive substitution rule: from each row of the current structure, identify the operator with the fewest occurrences, denoted X, and replace it with a symmetric pattern $YXYXY$, where Y corresponds to the next operator in the sequence. This recursive procedure can be used to systematically construct higher-order splitting methods while tracking the number of exponential terms. This process iteratively grows the composition while preserving symmetry and operator balance, enabling systematic construction of higher-order methods with controlled exponential complexity.

$N = 2$; 5 terms: $BABAB$
$N = 3$; 13 terms: $B\big[CACAC\big]B\big[CACAC\big]B$
$N = 4$; 25 terms: $\big[DBDBD\big]\big[CACAC\big]\big[DBDBD\big]\big[CACAC\big]\big[DBDBD\big]$
$N = 5$; 41 terms: $\big[DBDBD\big]C[EAEAE]C[EAEAE]C\big[DBDBD\big]$
$C[EAEAE]C[EAEAE]C\big[DBDBD\big]$.

The structure for a fourth order splitting for dimensions $N \geq 2$ is obtained as follows:
$N = 2$, 7 terms: $BABABAB$
$N = 3$, 25 terms: $B\big[CACACAC\big]B\big[CACACAC\big]B\big[CACACAC\big]B$
$N = 4$, 49 terms: $\big[DBDBDBD\big]\big[CACACAC\big]\big[DBDBDBD\big]\big[CACACAC\big]$
$\big[DBDBDBD\big]\big[CACACAC\big]\big[DBDBDBD\big]$.

This method of observing the number of required exponential terms can be modeled through a simple algorithm.

Algorithm 4.1 Algorithm for generating the number of exponential terms for $N > 2$

1: **Input:** Let x be the number of exponential terms for $N = 2$
2: Initialize List1 with $\left[\frac{x-1}{2}, \frac{x+1}{2}\right]$
3: **for** $i = 1$ to $N - 1$ **do**
4: Sort List1 in ascending order
5: Let a be the first element of List1
6: Remove a from List1
7: Append $a \times \frac{x-1}{2}$ and $a \times \frac{x+1}{2}$ to List1
8: Let Sum be the sum of elements in List1
9: **Print:** Iteration i: Total number of terms = Sum
10: **end for**

Table 1: Number of exponential terms involved in N-dimensional splittings of order p

Method	**p**	**N = 2**	**N = 3**	**N = 4**	**N = 5**	**N = 6**	**N = 7**	**N = 8**
Lie-Trotter	**1**	2	3	4	5	6	7	8
Strang	**2**	3	5	7	9	11	13	15
3rd	**3**	5	13	25	41	65	89	121
4th	**4**	7	25	49	103	175	247	343
6th	**6**	17	145	289	1313	2465	3617	4913
8th	**8**	55	1513	3025	42391	83215	124039	166375
10th	**10**	513	131585	263189	33817601	67634689		
12th	**12**	2049	2099201	4198401				
14th	**14**	8193	33562625					

As we investigate the number of exponential terms required for various higher-order methods applied to higher-dimensional systems, we observe that the number of terms grows rapidly with both the dimension and the order of the method. This substantial increase leads to greater complexity in the approximation. In this work, we investigate the two-dimensional case up to **14th** order and the three-dimensional case up to **sixth**-order, as discussed in detail in Section 5. These examples demonstrate that the accuracy of the approximation improves systematically with the order of the method.

Remark 4.11. In the corresponding table, some of the entries for the number of exponential terms are omitted, as the quantity becomes exceedingly large for higher-order methods in higher dimensions. Although these values are computable, listing them is unnecessary for practical purposes and would not add significant insight.

Our method can be extended to higher-dimensional systems and higher-order techniques. Future work will focus on refining algorithms to efficiently handle the complexity of exponential terms, expanding the framework's applicability to a broader range of problems in numerical analysis and dynamical systems.

4.4. Algorithms. All of the methods mentioned above for solving autonomous second-order and first-order problems can be generalized into a straightforward method for solving systems of differential equations via separation of variables. In order to solve a 2-D initial value problem

$$(x'(t), y'(t)) = (F_1(x(t), y(t)), F_2(x(t), y(t))), \quad (x(0), y(0)) = (x_0, y_0) \tag{4.27}$$

we follow the following remark.

Remark 4.12. Let $F = (F_1, F_2) : \mathbb{R}^2 \supset \Omega \to \mathbb{R}^2$, where Ω is assumed closed. If $x'(t) = F(x(t))$, $x(0) = x$, has unique, global, jointly continuous solutions $\sigma(t, x) \in \Omega$ for all $x = (x_1, x_2) \in \Omega$, then

$$T(t)g(x) := g(\sigma(t, x)) = e^{t\mathcal{K}}g(x) = e^{t(\mathcal{K}_1+\mathcal{K}_2)}g(x)$$

is bi-continuous on $C_b(\Omega)$, where $\mathcal{K}_i g(x) := F_i(x)g_{x_i}(x)$, $e^{t\mathcal{K}_1}g(x) = g(\sigma(t, x_1), x_2)$, $e^{t\mathcal{K}_2}g(x) = g(x_1, \gamma(t, x_2))$. Here, $\sigma(t, x_1)$ solves the frozen problem $x'(t) = F_1(x(t), x_2), x(0) = x_1$, and $\gamma(t, x_2)$ solves the frozen problem $x'(t) = F_2(x_1, x(t)), x(0) = x_2$. Thus, applying contractions $V_1(t) = e^{t\mathcal{K}_2}e^{t\mathcal{K}_1}$ and $V_2(t) = e^{\frac{t}{2}\mathcal{K}_1}e^{t\mathcal{K}_2}e^{\frac{t}{2}\mathcal{K}_1}$ such that

$$g(\sigma(t, x)) = T(t)g(x) = \lim_{n\to\infty} \left(V(\frac{t}{n})\right)^n g(x) = \lim_{n\to\infty} g(x_n(t, x)),$$

where by Proposition 4.3, $\sigma(t, x) = \lim_{n\to\infty} x_n(t, x)$. This is equivalent to solving

$$(x'(t), y'(t)) = (F_1(x(t), y(t)), F_2(x(t), y(t))), (x(0), y(0)) = (x, y)$$

via separation of variables after splitting into first-order sub-problems. We first freeze the variable y and solve the first-order problem $x'(t) = F_1(x(t), y)$, $x(0) = x_0$ with solution $x(t) = \sigma_y(t, x_0)$. Then, we freeze x and solve $y'(t) = F_2(x, y(t))$, $y(0) = y_0$ with solution $y(t) = \gamma_x(t, y_0)$. Finally, we combine the solutions of the sub-problems using the Lie-Trotter and Strang methods, where

$$e^{t\mathcal{K}_1}g(x, y) = g(\sigma_y(t, x), y) \text{ and } e^{t\mathcal{K}_2}g(x, y) = g(x, \gamma_x(t, y)).$$

(a) To apply Lie-Trotter $V_1(t)$, we use the following simple algorithm with starting values $x_0 := x$, $y_0 := y$. Then, for $0 \leq k \leq n-1$, we use the iterative process

$$\begin{aligned} &(1) \quad x_{k+1} = \sigma_{y_k}\left(\frac{t}{n}, x_k\right) \\ &(2) \quad y_{k+1} = \gamma_{x_{k+1}}\left(\frac{t}{n}, y_k\right). \end{aligned}$$

Then, $x_n = x_n(t) \approx x(t)$ $y_n = y_n(t) \approx y(t)$ with approximation order $C\frac{t^2}{n}$.

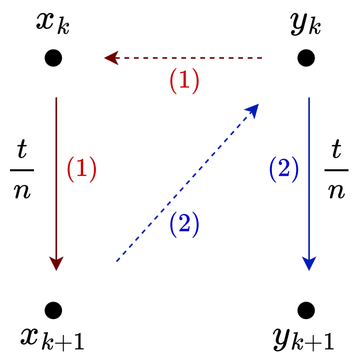
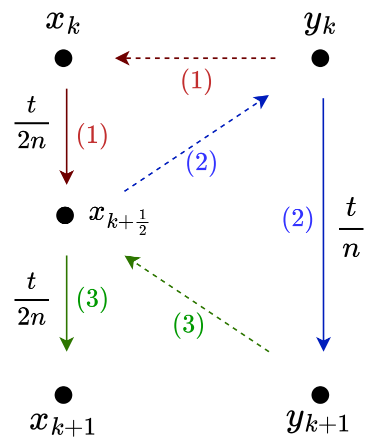


Figure 1: Graphical representation of Lie-Trotter $V_1(t)$.

The graphical representation of the Lie-Trotter operator, $V_1(t)$, is presented as follows: we begin with (x_k, y_k) and move through two main steps in each iterations. For step (1), we keep y_k fixed (indicated by dashed horizontal arrow) and solve only for x, moving vertically from x_k to x_{k+1} over a short time $\frac{t}{n}$. For step (2), we keep the newly computed x_{k+1} fixed (shown by dashed diagonal arrow) and update y, moving vertically from y_k to y_{k+1} over the same time step $\frac{t}{n}$. Then together they form one full updated in the algorithm, taking us from (x_k, y_k) to (x_{k+1}, y_{k+1}).
(b) To apply Strang $V_2(t)$, we use the following simple algorithm with starting values $x_0 := x$, $y_0 := y$. Then, for $0 \leq k \leq n-1$, we use the iterative process

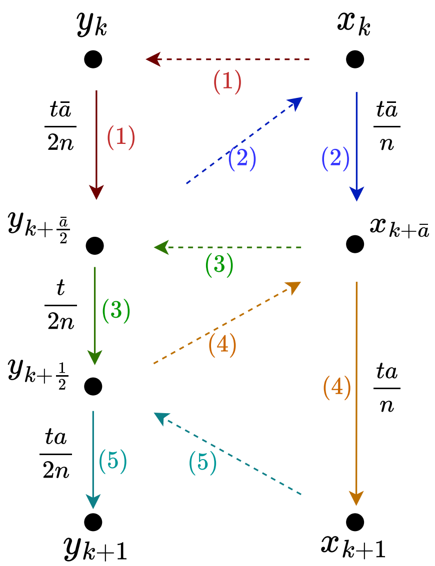
$$
\begin{aligned}
&(1) \quad x_{k+\frac{1}{2}} &&= \sigma_{y_k}\Big(\frac{t}{2n}, x_k\Big),\\
&(2) \quad y_{k+1} &&= \gamma_{x_{k+\frac{1}{2}}}\Big(\frac{t}{n}, y_k\Big),\\
&(3) \quad x_{k+1} &&= \sigma_{y_{k+1}}\Big(\frac{t}{2n}, x_{k+\frac{1}{2}}\Big).
\end{aligned}
$$



Then, $x_n = x_n(t) \approx x(t)$ $y_n = y_n(t) \approx y(t)$ with approximation order $C\frac{t^3}{n^2}$.

(c) To apply the third order $V_3(t)$ given by Proposition 4.7, we use the following simple algorithm with starting values $x_0 := x$, $y_0 := y$. Then, for $0 \leq k \leq n-1$, we use the iterative process

$$
\begin{aligned}
&(1) \quad y_{k+\frac{\bar{a}}{2}} &&= \gamma_{x_k}\Big(\frac{t\bar{a}}{2n}, y_k\Big),\\
&(2) \quad x_{k+\bar{a}} &&= \sigma_{y_{k+\frac{\bar{a}}{2}}}\Big(\frac{t\bar{a}}{n}, x_k\Big),\\
&(3) \quad y_{k+\frac{1}{2}} &&= \gamma_{x_{k+\bar{a}}}\Big(\frac{t}{2n}, y_{k+\frac{\bar{a}}{2}}\Big),\\
&(4) \quad x_{k+1} &&= \sigma_{y_{k+\frac{1}{2}}}\Big(\frac{ta}{n}, x_k\Big),\\
&(5) \quad y_{k+1} &&= \gamma_{x_{k+1}}\Big(\frac{ta}{2n}, y_{k+\frac{1}{2}}\Big).
\end{aligned}
$$



Then, $x_n = x_n(t) \approx x(t)$ $y_n = y_n(t) \approx y(t)$ with approximation order $C\frac{t^4}{n^3}$ given $a = \frac{1}{2} + i\frac{\sqrt{3}}{6}$.

In addition, all the methods mentioned above for solving autonomous three-dimensional problems can be generalized into a straightforward method for solving systems of differential equations via separation of variables, as explained below.

Remark 4.13. Let $F = (F_1, F_2, F_3) : \mathbb{R}^3 \supset \Omega \to \mathbb{R}^3$, Ω closed. If $u'(t) = F(u(t))$, $u(0) = x$, has unique, global, jointly continuous solutions $\sigma(t,x) \in \Omega$ for all, $x = (x_1, x_2, x_3) \in \Omega$, then

$$T(t)g(x) := g(\sigma(t,x)) = e^{t\mathcal{K}}g(x) = e^{t(\mathcal{K}_1+\mathcal{K}_2+\mathcal{K}_3)}g(x)$$

is bi-continuous on $C_b(\Omega)$, where $\mathcal{K}_i g(x) := F_i(x)g_{x_i}(x)$. Define
$e^{t\mathcal{K}_1}g(x) = g(\sigma(t,x_1), x_2, x_3)$, $e^{t\mathcal{K}_2}g(x) = g(x_1, \gamma(t,x_2), x_3)$, and $e^{t\mathcal{K}_3}g(x) = g(x_1, x_2, \tau(t,x_3))$. Here, $\sigma(t,x_1)$ solves the frozen problem $x'(t) = F_1(x(t), x_2, x_3), x(0) = x_1$, $\gamma(t,x_2)$ solves the frozen problem $x'(t) = F_2(x_1, x(t), x_3), x(0) = x_2$, and $\tau(t,x_3)$ solves the frozen problem $x'(t) = F_3(x_1, x_2, x(t)), x(0) = x_3$. Thus, applying contractions $V_1(t) = e^{t\mathcal{K}_3}e^{t\mathcal{K}_2}e^{t\mathcal{K}_1}$ such that

$$g(\sigma(t,x)) = T(t)g(x) = \lim_{n\to\infty}\left(V(\frac{t}{n})\right)^n g(x) = \lim_{n\to\infty} g(x_n(t,x)),$$

where by Proposition 4.3, $\sigma(t,x) = \lim_{n\to\infty} x_n(t,x)$. This is equivalent to solving

$$(x'(t), y'(t), z'(t)) = (F_1(x(t), y(t), z(t)), F_2(x(t), y(t), z(t)), F_3(x(t), y(t), z(t))),$$

given $(x(0), y(0), z(0)) = (x, y, z)$, via separation of variables after splitting into the following first-order sub-problems. We first freeze the variables y and z and solve the first-order problem

$$x'(t) = F_1(x(t), y, z),\ x(0) = x_0 = x$$

with solution $x(t) = \sigma_{y,z}(t,x)$, then freeze x and z to solve

$$y'(t) = F_2(x, y(t), z),\ y(0) = y_0 = y$$

with solution $y(t) = \gamma_{x,z}(t,y)$, and then freeze x and y to solve

$$z'(t) = F_3(x, y, z(t)),\ z(0) = z_0 = z$$

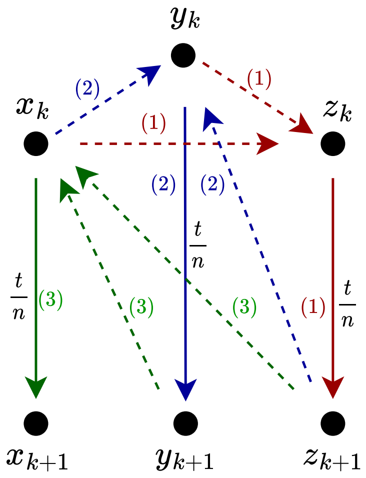
with solution $z(t) = \tau_{x,y}(t,z)$. Finally, we combine the solutions of the sub-problems with a product formula like Lie-Trotter $V_1(t)$ or $VS(t)$, where

$$e^{t\mathcal{K}_1}g(x,y,x) = g(\sigma_{y,z}(t,x), y, z), \quad e^{t\mathcal{K}_2}g(x,y,z) = g(x, \gamma_{x,z}(t,y), z), \text{ and}$$

$$e^{t\mathcal{K}_3}g(x,y,z) = g(x, y, \tau_{x,y}(t,z)).$$

To apply Lie-Trotter $V_1(t)$,we use the following simple algorithm with starting values $x_0 := x$, $y_0 := y$, $z_0 := z$. Then, for $0 \le k \le n-1$, we use the iterative process

$$
\begin{aligned}
&(1) \quad z_{k+1} &&= \tau_{x_k,y_k}(\frac{t}{n}, z_k),\\
&(2) \quad y_{k+1} &&= \gamma_{x_k,z_{k+1}}(\frac{t}{n}, y_k),\\
&(3) \quad x_{k+1} &&= \sigma_{y_{k+1},z_{k+1}}(\frac{t}{n}, x_k).
\end{aligned}
$$



Then, $x_n = x_n(t) \approx x(t)$, $y_n = y_n(t) \approx y(t)$, $z_n = z_n(t) \approx z(t)$ with approximation order $C\frac{t^2}{n}$.

In Appendices B and C, we provide additional algorithms illustrating how the Strang splitting and third-order approximations can be applied to three-dimensional problems. Throughout this work, we employ all of the algorithms discussed to numerically approximate solutions to various systems. Moreover, even algorithms that are not explicitly presented here can be systematically constructed following similar procedures, highlighting the flexibility and generality of our approach.

5. Numerical Experiments.

Example 5.1 (Lotka-Volterra).

The Lotka–Volterra model describes the interaction between predator and prey populations over time. It captures how prey grow in the absence of predators, while predators depend on prey for survival. This interaction leads to cyclical population dynamics governed by a nonlinear system of differential equations:

$$
\begin{aligned}
x'(t) &= \alpha x(t) - \beta x(t)y(t), \quad x(0) = x_0 = x\\
y'(t) &= \delta x(t)y(t) - \tau y(t), \quad y(0) = y_0 = y
\end{aligned}
$$

Step 1: *Solve the first-order system via separation of variables.*

a) Freeze y: $\quad x'(t) = x(t)(\alpha - \beta y)$

$$\Rightarrow x(t) = \sigma_y(t, x) = xe^{t(\alpha-\beta y)}$$

b) Freeze x: $\quad y'(t) = y(t)(\delta x - \tau)$

$$\Rightarrow y(t) = \gamma_x(t, y) = ye^{t(\delta x-\tau)}$$

Step 2: *Finally, to approximate the solutions, we can apply the Lie-Trotter $V_1(t)$ method (see part (a), Remark 4.12).*

We then obtain the following numerical approximation of the solutions for the given initial conditions: $\alpha = 0.5$, $\beta = 0.02$, $\delta = 0.01$, $\tau = 0.1$, $x_0 = 100$, $y_0 = 10$. Consider the number of iterations $n = 1000$ and the total time $t = 100$.

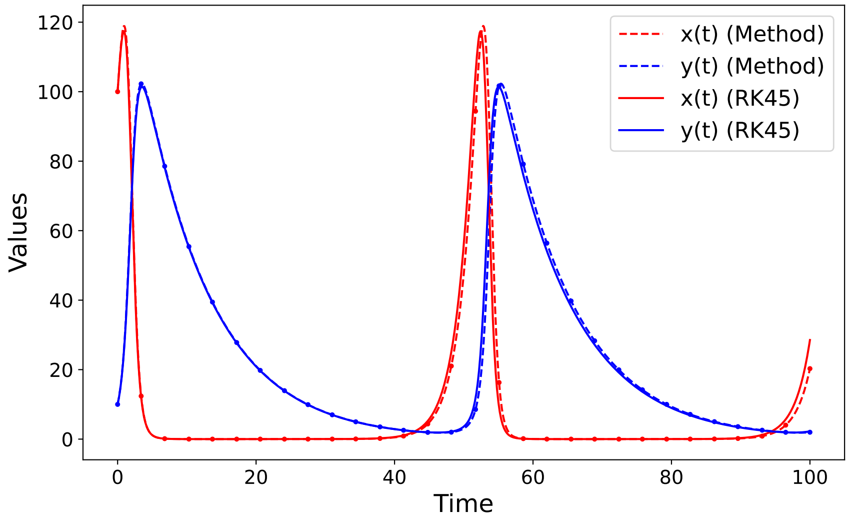


Figure 2: Comparison of Lie-Trotter and Runge-Kutta (RK45) solution ($t = 100, n = 1000$)

Similarly, we can apply the Strang splitting $V_2(t)$ method (Part (b), Remark 4.12) to approximate the solution and compare it against the RK45 (Runge-Kutta) method.

To compare the list of approximated coordinates obtained from our method with those computed by the RK45 method at a fixed time t, we apply the Root Mean Square Error (RMSE) as a metric to measure the overall discrepancy. To ensure that the RK45 solution serves as a highly accurate reference, we set both the relative and absolute tolerances to a very small value, specifically 10^{-16}. This choice guarantees that the RK45 approximation is sufficiently precise for meaningful comparison. After computing the RMSE values, we will organize them into a table for various test cases and analyze the results to evaluate the performance and accuracy of our proposed method. The formula for RMSE is given below:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\Big((x_i^{approx} - x_i^{RK45})^2 + (y_i^{approx} - y_i^{RK45})^2\Big)}.$$

From the Table 2, we observe that for $n = 100$ iterations, the lowest RMSE is achieved using the 12th-order method. As the number of iterations increases, lower-order methods become sufficient to achieve similarly low RMSE values. Specifically, for $n = 1000$, the 10th-order method yields the lowest RMSE, and for $n = 10000$, only the 6th-order method is

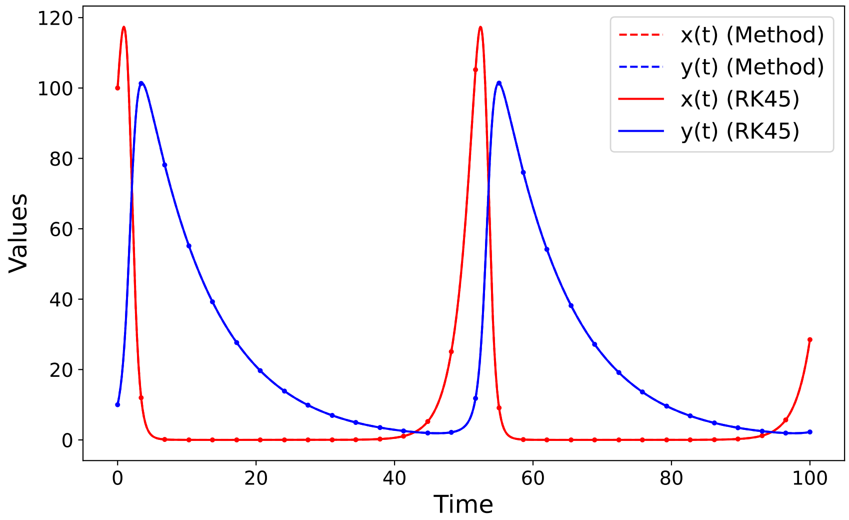


Figure 3: Comparison of Strang and Runge-Kutta (RK45) solution ($t = 100, n = 1000$)

Table 2: Root Mean Square Error (RMSE) against RK45 method with tolerance 10^{-16}

n	**Lie-Trotter**	**Strang**	**3rd**	**6th**	**8th**	**10th**	**12th**	**14th**
100	33.015	1.883	1.47	0.0008	$7.0E^{-8}$	$5.77E^{-12}$	$\mathbf{7.75E^{-13}}$	$1.01E^{-11}$
1000	4.159	0.017	$2.73E^{-05}$	$2.33E^{-11}$	$1.57E^{-11}$	$\mathbf{1.43E^{-11}}$	$9.32E^{-10}$	$1.41E^{-09}$
10000	0.415	0.0002	$2.02E^{-09}$	$\mathbf{3.28E^{-11}}$	$7.9E^{-11}$	$1.32E^{-09}$	$1.34E^{-09}$	$1.29E^{-08}$

needed. This trend confirms that increasing the number of iterations improves the accuracy of the approximation, and higher-order methods further enhance this accuracy, particularly when the number of iterations is limited. Therefore, both increasing the number of iterations and employing higher-order methods play complementary roles in achieving more precise solutions.

Example 5.2 (Van der Pol Oscillator).

The Van der Pol oscillator models nonlinear systems with amplitude-dependent damping, producing self-sustained oscillations that converge to a stable limit cycle. Originally used for electrical circuits, it remains a key example for studying nonlinear behavior such as relaxation oscillations and bifurcations. The Van der Pol oscillator is described by the second-order nonlinear differential equation:

$$x''(t) + (x(t)^2 - 1)x'(t) + x(t) = 0, \quad x(0) = x_0 = x, \quad x'(0) = y$$

has a unique, global solution $t \to x(t)$ *for all* $x, y \in \mathbb{R}^2$. *Generalized Van der Pol* $\to$ *Liénard system:*

$$x''(t) - a(x(t))x'(t) - b(x(t)) = 0, \quad x(0) = x_0 = x, \quad x'(0) = y.$$

Define $y(t) = x'(t)$, $F_1(x, y) := y$ and $F_2(x, y) = a(x)y + b(x)$. Then the equivalent first-order autonomous system is given by

$$x'(t) = F_1(x(t), y(t)) = y(t), \quad x(0) = x_0 = x$$

$$y'(t) = F_2(x(t), y(t)) = a(x(t))y(t) + b(x(t)), \quad y(0) = y_0 = y$$

Step 1: *Solve the first-order system via separation of variables.*

a) Freeze y: $\quad x'(t) = y, \quad x(0) = x$

$$\Rightarrow x(t) = \sigma_y(t, x) = yt + x$$

b) Freeze x: $\quad y'(t) = a(x)y(t) + b(x), \quad y_0 = y$

$$\Rightarrow y(t) = \gamma_x(t, y) = b(x)\frac{(e^{ta(x)} - 1)}{a(x)} + ye^{ta(x)}$$

Step 2: *Finally, to approximate the solutions, we can apply the Lie-Trotter $V_1(t)$ method (Part (a), Remark 4.12).*

We then obtain the following numerical approximation of the solutions for the given initial conditions: $x_0 = -0.2$, $y_0 = 0$, $a(x) = 1 - x^2$, and $b(x) = -x$. We observe the graph up to a total time $t = 25$.

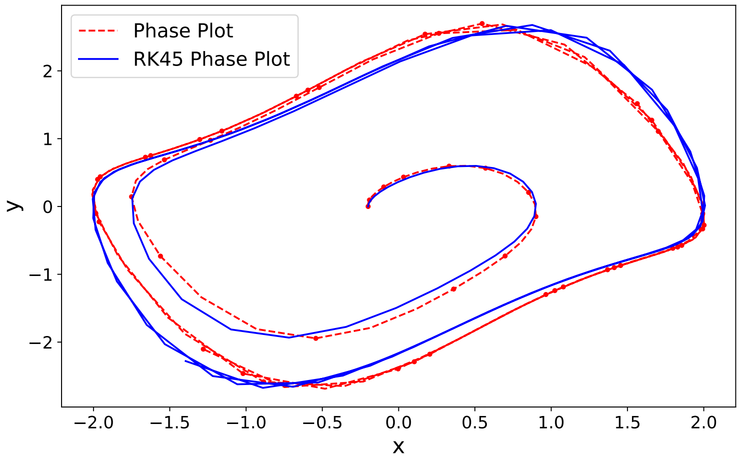


Figure 4: Comparison of Lie-Trotter (Blue) vs RK45 (Red) ($t = 25, n = 125$)

Similarly, we can apply the Strang splitting $V_2(t)$ method (see part (b), Remark 4.12) to approximate the solution and compare it against the RK45 (Runge-Kutta) method. We observe that the accuracy of the approximation improves with higher-order discretization.

The initial conditions are as listed above and $t = 25$. The Table 3 shows that for $n = 125$ iterations, the minimum RMSE is obtained using the 10th-order method. As the number of

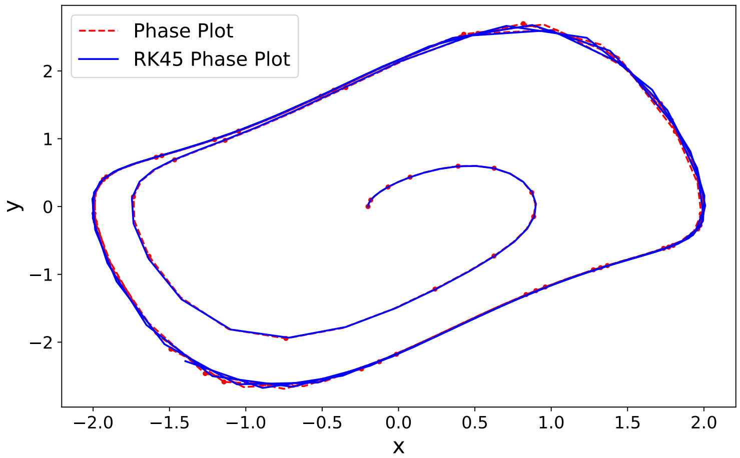


Figure 5: Comparison of Strang (Blue) vs RK45 (Red) ($t = 25, n = 125$)

Table 3: Root Mean Square Error (RMSE) against RK45 method with tolerance 10^{-16}

n	**Lie-Trotter**	**Strang**	**3rd**	**6th**	**8th**	**10th**	**12th**	**14th**
125	0.111	0.071	0.001	$2.99E^{-08}$	$5.96E^{-13}$	$\mathbf{1.67E^{-13}}$	$8.92E^{-13}$	$8.96E^{-12}$
500	0.031	0.004	$6.84E^{-06}$	$4.70E^{-12}$	$\mathbf{3.64E^{-13}}$	$1.50E^{-12}$	$1.11E^{-11}$	$8.49E^{-11}$
1000	0.016	0.001	$4.56E^{-07}$	$\mathbf{1.80E^{-13}}$	$7.87E^{-12}$	$4.47E^{-12}$	$3.48E^{-11}$	$1.74E^{-10}$

iterations increases, lower-order methods become sufficient to achieve comparable accuracy. In particular, for $n = 500$, the eighth-order method yields the lowest RMSE, and for $n = 1000$, the 6th-order method suffices. This pattern indicates that both increasing the number of iterations and raising the order of the method contribute to improving the approximation. Higher-order methods are especially beneficial when the number of iterations is relatively small, while with sufficiently many iterations, even lower-order methods can produce highly accurate results. Thus, the number of iterations and the order of the method work together to enhance precision.

Example 5.3 (Lorenz System).
The Lorenz system is a classic example of chaos arising from simple deterministic rules. Originally developed to model atmospheric convection, it is governed by three nonlinear differential equations describing fluid flow. Known for its sensitivity to initial conditions, small variations can lead to drastically different outcomes, a hallmark of chaos. The system's solutions exhibit the characteristic butterfly-shaped Lorenz attractor in three-dimensional space. For parameters α, ρ, and β, the system is defined by:

$$
\begin{aligned}
x'(t) &= \alpha(y(t) - x(t)), & x_0 &= x, \\
y'(t) &= x(t)(\rho - z(t)) - y(t), & y_0 &= y, \\
z'(t) &= x(t)y(t) - \beta z(t), & z_0 &= z.
\end{aligned}
$$

Step 1: *Solve the first order Lorenz system via separation of variables*

a) Freeze y, z: $\quad x'(t) = F_1(x(t), y, z) = \alpha(y - x(t)), \quad x_0 = x$

$$\Rightarrow x(t) = \sigma_{y,z}(t, x) = y(1 - e^{-\alpha t}) + xe^{-\alpha t}$$

b) Freeze x, z: $\quad y'(t) = F_2(x, y(t), z) = x(\rho - z) - y(t), \quad y_0 = y$

$$\Rightarrow y(t) = \gamma_{x,z}(t, y) = x(\rho - z)(1 - e^{-t}) + ye^{-t}$$

c) Freeze x, y: $\quad z'(t) = F_3(x, y, z(t)) = xy - \beta z(t), \quad z_0 = z$

$$\Rightarrow z(t) = \tau_{x,y}(t, z) = \frac{xy}{\beta}(1 - e^{-\beta t}) + ze^{-\beta t}$$

Step 2: *Finally, to approximate the solutions, we can apply the Lie-Trotter $V_1(t)$ method (see Remark 4.13). We then obtain the following numerical approximation of the solutions for the given initial conditions: $(\alpha, \rho, \beta) = (10, 28, 8/3)$, $(x_0, y_0, z_0) = (1, 1, 1)$. We observe the graph and compare it with the RK45 method.*

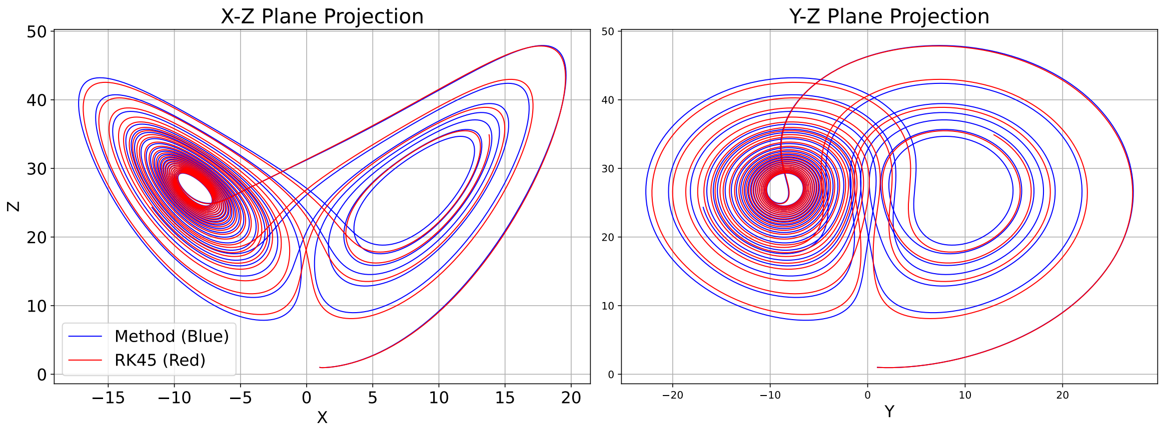


Figure 6: Comparison of Lie-Trotter (Blue) vs RK45 (Red) $(t = 20, n = 20000)$.

Similarly, we apply the Strang splitting method to approximate the solution and compare it against the RK45 (Runge-Kutta) method. We observe that the accuracy of the approximation improves with higher-order discretization.

As we have shown in the previous examples, we compute the Root Mean Square Error (RMSE) to compare the approximated solution with the RK45 method for this three-dimensional system. The RMSE provides a quantitative measure of the overall difference between the two solutions across all three coordinates (x, y, and z) over the time interval considered. By calculating the RMSE, we can systematically evaluate the accuracy of the approximated method relative to the highly accurate RK45 benchmark. This allows us to assess the effectiveness of our approach in higher-dimensional settings as well. For our comparison we use the initial condition as above with time $t = 20$ and RK45 method with relative and absolute tolerance of 10^{-16}.The formula for RMSE is given below:

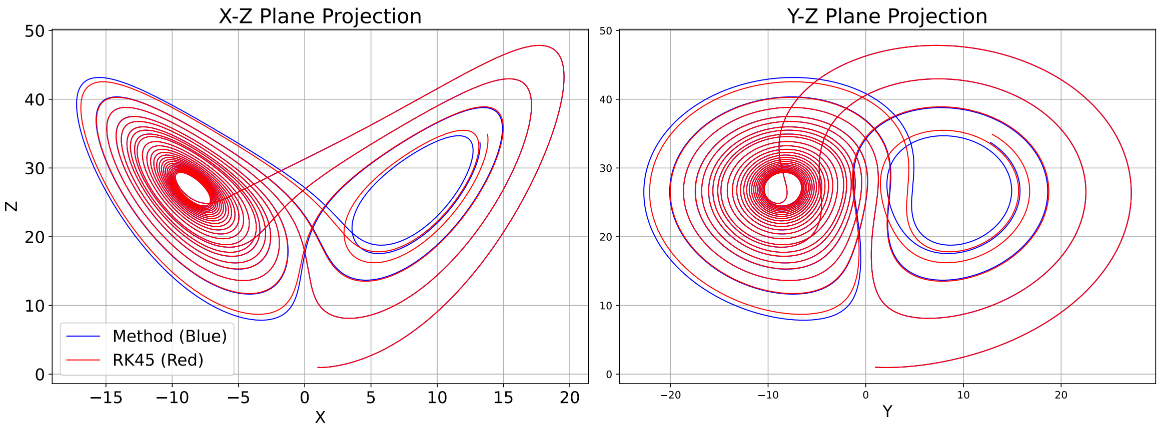


Figure 7: Comparison of Strang (Blue) vs RK45 (Red) $(t = 20, n = 20000)$

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left((x_i^{\text{approx}} - x_i^{\text{RK45}})^2 + (y_i^{\text{approx}} - y_i^{\text{RK45}})^2 + (z_i^{\text{approx}} - z_i^{\text{RK45}})^2\right)}$$

Table 4: Root Mean Square Error (RMSE) against RK45 method with tolerance 10^{-16}

n	**Lie-Trotter**	**Strang**	**3rd**	**6th**
1000	15.486	10.087	7.569	$\mathbf{3.23E^{-06}}$
20000	12.554	1.245	$1.85E^{-05}$	$\mathbf{7.48E^{-08}}$
100000	10.367	0.041	$\mathbf{2.27E^{-08}}$	$2.75E^{-07}$

The Table 4 shows that for $n = 1000$ iterations, the minimum RMSE is achieved using the 6th-order method. Similarly, for $n = 20000$, the 6th-order method again yields the lowest RMSE, while for $n = 100000$, the third-order method suffices. This pattern indicates that both increasing the number of iterations and increasing the order of the method contribute to improving the approximation. Higher-order methods are particularly advantageous when the number of iterations is relatively small, whereas with a sufficiently large number of iterations, even lower-order methods can produce highly accurate results. Thus, the number of iterations and the order of the method work together to enhance the precision of the solution.

6. Conclusion and future directions. The numerical results in Tables 2, 3, and 4 demonstrate that approximation accuracy, measured by RMSE, depends on both the number of iterations n and the order of the splitting method. In the case of the Lotka–Volterra system (Table 2), higher-order schemes—such as the 12th-order method—achieve the lowest RMSE for small n. For the Van der Pol equation (Table 3), similar behavior is observed, with the eighth-order method performing best at $n = 500$ and the sixth-order method excelling at

$n = 1000$. In the chaotic Lorenz system (Table 4), the third-order method becomes highly accurate as n reaches 100,000. This trend highlights a practical trade-off between iteration count and method order, guiding efficient choices in computational settings. Compared to classical schemes such as the Runge–Kutta method (e.g., RK45 with the absolute and relative tolerances of 10^{-16}), the splitting method is not only competitive in accuracy but also more computationally efficient. This efficiency arises from decomposing the original problem into smaller sub-problems that can be solved independently using separation of variables, significantly reducing the computational cost, especially for high-dimensional systems.
These results demonstrate a complementary relationship: increasing the number of iterations improves precision, while higher-order methods enhance accuracy when iteration counts are limited. Therefore, both increasing the number of iterations and employing higher-order methods play complementary roles in achieving more precise solutions.

Several directions for future research can be identified. In Definitions 3.1, 3.2, and Proposition 3.4, the analysis was restricted to autonomous flows. A natural extension of this framework would involve the generalization to non-autonomous flows. Moreover, it may be possible to broaden the scope of the theory to encompass partial differential equations (PDEs).

Within the present context, we define the global flow $\sigma(t,x)$ for all $t \geq 0$ and $x \in \Omega$ in Definition 3.1, and associate it with the Koopman operator $T(t)g(x) = g(\sigma(t,x))$, which acts linearly on a function space $\mathcal{F}$ or on a $T(t)$-invariant subspace. However, in the case of a *local* flow—i.e., when the flow is only defined for $t \in [0,T)$ with $T < \infty$—the corresponding family $T(t)g(x) = g(\sigma(t,x))$ no longer fits within the classical framework of semigroup theory, [29].

To rigorously address this issue, it becomes necessary to introduce a stopping time framework, along with appropriate adjustments to the function space and the associated semigroup structure. These modifications are fundamental for extending the Koopman–Lie framework to the setting of local flows. In subsequent work, we shall direct our attention to a detailed analysis of local flow dynamics.

7. Reproducibility of computational results. This work has been prepared with a strong commitment to reproducibility. All code and data necessary to replicate the results presented in this paper are publicly available at: https://github.com/odeSolver/Operator-Splitting-Methods. This paper is intended for submission to a SIAM journal and will be eligible for the SIAM Reproducibility Badge: Code and Data Available.

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Appendix A. Proof of Proposition 4.3.

Proof. Clearly, (a) implies (b). If (b) holds, it follows that x_n is bounded. If not, there would be a subsequence x_j of x_n such that $|x_j| \to \infty$. Now define $g_0(x) := \frac{1}{1+|x|}$. Then $g_0(x_i) \to 0$ and $g_0(x_i) \to g(x) > 0$ as $i \to \infty$, which is a contradiction. Thus, if (b) holds, there exists $M > 0$ such that $|x| \leq M$ and $|x_n| \leq M$ for all n. Now let $P_j(x) := x_j$, where x_j is the j-th coordinate of x. Define the truncated coordinate function as $f_j(x) = (x_j \wedge M) \vee -M$. Then the truncated coordinate functions are bounded, continuous functions, and therefore $f_j(x_n) = P_j(x_n) \to f_j(x) = P_j(x)$ for all $1 \leq j \leq N$. Thus, x_n converges coordinate-wise to x

and, therefore, x_n converges to x.

Appendix B. Algorithm for three-dimensional Strang method.

To apply Strang $V_2(t)$ (see Equation 4.15) for three-dimensional system, we use the following the algorithm with starting values $x_0 := x$, $y_0 := y$, $z_0 := z$. Then, for $0 \leq k \leq n-1$, we use the iterative process to obtain the solution x_n and y_n.

$$
\begin{aligned}
z_{k+\frac{1}{2}} &= \tau_{y_k, z_k}(\frac{t}{2n}, z_k),\\
y_{k+\frac{1}{2}} &= \gamma_{x_k, z_{k+\frac{1}{2}}}(\frac{t}{2n}, y_k),\\
x_{k+1} &= \sigma_{y_{k+\frac{1}{2}}, z_{k+\frac{1}{2}}}(\frac{t}{n}, x_k),\\
y_{k+1} &= \gamma_{x_{k+1}, z_{k+\frac{1}{2}}}(\frac{t}{2n}, y_{k+\frac{1}{2}}),\\
z_{k+1} &= \tau_{y_{k+1}, z_{k+1}}(\frac{t}{2n}, z_{k+\frac{1}{2}}).
\end{aligned}
$$

Appendix C. Algorithm for three-dimensional third order method.

The exponential splitting method explained in the earlier sections provides a general approach for extending the method from the two-dimensional problem to higher dimensions. The third-order equation (see Equation 4.8) involves 5 exponential terms, and from Table 1, we observe that the three-dimensional method involves 13 terms. To apply the third order $V_3(t)$ for the three dimensional problem, we use the following algorithm with the initial values $x_0 := x$, $y_0 := y$, $z_0 := z$. Then, for $0 \leq k \leq n-1$ and $a = \frac{1}{2} + i\frac{\sqrt{3}}{6} = 0.5 + 0.28875i$, with $\bar{a}$ being its conjugate, we use the iterative process below to obtain the solution x_n, y_n, and z_n.

$$
\begin{aligned}
&\text{Step 1:} && y_p = \gamma_{x_k,z_k}(\frac{t\bar{\alpha}}{2n}, y_k)\\
&\text{Step 2:} && z_p = \tau_{x_k,y_p}(\frac{t(\bar{\alpha})^2}{2n}, z_k)\\
&\text{Step 3:} && x_p = \sigma_{y_p,z_p}(\frac{t(\bar{\alpha})^2}{n}, x_k)\\
&\text{Step 4:} && z_q = \tau_{x_p,y_p}(\frac{t\bar{\alpha}}{2n}, z_p)\\
&\text{Step 5:} && x_q = \sigma_{y_p,z_q}(\frac{t\alpha\bar{\alpha}}{n}, x_p)\\
&\text{Step 6:} && z_r = \tau_{x_q,y_p}(\frac{t\alpha\bar{\alpha}}{2n}, z_q)\\
&\text{Step 7:} && y_q = \gamma_{x_q,z_r}(\frac{t}{2n}, y_p)\\
&\text{Step 8:} && z_s = \tau_{x_q,y_q}(\frac{t\alpha\bar{\alpha}}{2n}, z_r)\\
&\text{Step 9:} && x_r = \sigma_{y_q,z_s}(\frac{t\alpha\bar{\alpha}}{n}, x_q)\\
&\text{Step 10:} && z_t = \tau_{x_r,y_q}(\frac{t\alpha}{2n}, z_s)\\
&\text{Step 11:} && x_{k+1} = \sigma_{y_q,z_t}(\frac{t\alpha^2}{n}, x_r)\\
&\text{Step 12:} && z_{k+1} = \tau_{x_{k+1},y_q}(\frac{t\alpha^2}{2n}, z_t)\\
&\text{Step 13:} && y_{k+1} = \gamma_{x_{k+1},z_{k+1}}(\frac{t\alpha}{2n}, y_q).
\end{aligned}
$$

Similarly, the algorithm for any higher-order exponential splitting methods, as discussed in Theorem 4.8, can be generated. Furthermore, by applying the idea from Section 4.3, the method can be extended from the two-dimensional problem to higher dimensions. The number of terms involved can be easily computed, and the complexity arising from higher-dimensional higher-order methods can be anticipated.

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