HIGH ORDER METHODS FOR IRREVERSIBLE EQUATIONS

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Abstract. In this work, we show high order splitting methods of integration without negative steps, allowing us to solve numerically irreversible problems, like reaction–diffusion equations. The methods consist in a suitable affine combinations of Lie-Trotter schemes with different steps. We prove convergence of this methods for a large class of semi-linear problems, that includes Hamiltonian and reaction-diffusion systems.

1. Introduction

We study the initial value problem

\[ u_t = A_0 u + A_1(u), \quad u(0) = u_0. \]  

(1)

where \( A_0 \) is a close operator densely defined in \( D(A_0) \subset H \), \( H \) is a Hilbert space, which generates a strongly continuous semi-group of operators. We assume that the nonlinear term \( A_1 : H \to H \) is a smooth application with \( A_1(0) = 0 \). In many problems of interest, the partial equations \( u_t = A_0 u \) and \( u_t = A_1(u) \) can be easily solved, which enable to find approximated solutions of the problem (1) applying in turn the flow associated to each partial problem.

A highly known example of this kind of problems is the nonlinear Schrödinger equation (NLS):

\[ u_t = i \nabla^2 u + i|u|^2 u, \]

where the partial flows associated to each term of the equation are given by

\[ \phi_0(t, u_0) = \exp(it \nabla^2)u_0, \]
\[ \phi_1(t, u_0) = \exp(it|u_0|^2)u_0. \]

2010 Mathematics Subject Classification. 65M12 (primary), and 35Q55, 35K57 (secondary).

Key words and phrases. splitting methods, irreversible dynamics, reaction-diffusion systems.

This work was partially supported by PIP 11220090100637 CONICET and MATH-Amsud 11MATH-02 "PNDW".

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which represent the evolution of a free particle and self–phase modulation respectively.

There exist many numerical integration methods for (1) based on this idea, the most known are the Lie–Trotter and Strang methods defined by

\[
\Phi_{\text{Lie}}(h, u_0) = \phi_1(h, \phi_0(h, u_0)), \\
\Phi_{\text{Strang}}(h, u_0) = \phi_0(h/2, \phi_1(h, \phi_0(h/2, u_0))),
\]

where \(h\) is the time step of the numerical integration. It can be proved that \(\Phi_{\text{Lie}}\) has order 1 and \(\Phi_{\text{Strang}}\) has order 2, being the order \(q\) the number of terms that match in the Taylor expansions of the real flow \(\phi\) of the equation (1) and the numerical method \(\Phi\). That is, the order is the greater natural number such that the truncation error verifies

\[
\|\phi(h, u_0) - \Phi(h, u_0)\|_\mathcal{H} \leq C(u_0)h^{q+1}
\]

for \(0 < h < h_\ast\). Under stability hypothesis for the method, we will show that in this case, the global error of the method goes to zero as \(h^q\).

In [12], [11] and [15], the authors present numerical examples for Hamiltonian systems of order \(q = 3, 4, 2n\) respectively, which are known as symplectic integrators. The general form of this methods is the following:

\[
\Phi_S(h) = \phi_1(b_m h) \circ \phi_0(a_m h) \circ \cdots \circ \phi_1(b_1 h) \circ \phi_0(a_1 h),
\]

with \(a_1 + \cdots + a_m = b_1 + \cdots + b_m = 1\). In the pioneering work of Ruth [12], a symplectic operator \(\Phi_S\) of order 3 is presented, taking \(a = (7/24, 3/4, -1/24)\) and \(b = (2/3, -2/3, 1)\). In [11] a symplectic operator of order 4 is considered, where

\[
a_1 = a_4 = \frac{1}{2(2 - 2^{1/3})}, \quad a_2 = a_3 = -\frac{2^{1/3} - 1}{2(2 - 2^{1/3})}, \\
b_1 = b_3 = \frac{1}{2 - 2^{1/3}}, \quad b_2 = -\frac{2^{1/3}}{2 - 2^{1/3}}, \quad b_4 = 0.
\]

In [15], Yoshida presents a systematic way to obtain integrators of arbitrary even order as follows: from the Baker–Campbell–Hausdorff formula, it can be set inductively

\[
\Phi_{S,2n+2}(h) = \Phi_{S,2n}(z_1 h) \circ \Phi_{S,2n}(z_0 h) \circ \Phi_{S,2n}(z_1 h),
\]

with \(z_0 + 2z_1 = 1\) and \(z_0^{2n+1} + z_1^{2n+1} = 0\). The total number of steps of the method of order \(q = 2n\) is \(S_T = 3^n\). Nevertheless, for order \(q = 6, 8\) there can be shown symplectic integrators with 8 and 16 steps respectively.
In the last years, many authors started the rigorous study of the convergence of the symplectic methods applied to Hamiltonian systems in infinite dimension. In [3] the NLS problem in dimension 2 is considered and it is proved the convergence of the Lie–Trotter and Strang methods in $L^2(\mathbb{R}^2)$ with order 1 and 2 respectively. In [7, 9] similar results are proved for the Gross-Pitaevskii equation given by:

$$iu_t = -\nabla^2 u + |x|^2 u + |u|^2 u.$$  

In both cases, it is needed the solutions to be derivable with respect to time, and therefore initial data in $D(A_0^k)$ is considered, where $A_0$ is the corresponding differential operator.

The symplectic methods with order $q > 2$ require some step to be negative, inhibiting its application to irreversible problems. As an example of these we have the reaction–diffusion systems:

$$u_t = D\nabla^2 u + N(u)$$

where $u(x, t) \in \mathbb{R}^d$, $D \in \mathbb{R}^{d \times d}$ is a positive diagonal matrix and $N$ is a smooth application in $\mathbb{R}^d$. It is natural to split the problem into the linear diffusion equation $u_t = D\nabla^2 u$ and the ordinary differential equation system given by $\dot{u} = N(u)$, where the diffusion problem is ill posed for negative times. For these kind of problems, implicit Runge–Kutta schemes can be used to integrate the system that arises from the spatial discretization, but these type of methods not only do not take advantage of the simplicity of the partial problem (as in the splitting setting) but also bring on the complicated treatment of pseudo differential operators.

In this work, we present a family of splitting type methods for arbitrary order with positive time step, that exploit the simplicity of the partial flows in non reversible problems. Here we describe the methods proposed: given the associated flows $\phi_j$ of the partial problems, we define the applications $\phi^+(h) = \phi_1(h) \circ \phi_0(h)$, $\phi^-(h) = \phi_0(h) \circ \phi_1(h)$ and $\phi_m^\pm(h) = \phi_1^\pm(h) \circ \phi_{m-1}^\pm(h)$, and consider the following methods:

$$\Phi(h) = \sum_{m=1}^s \gamma_m \phi_m^\pm(h/m) \quad \text{(asymmetric)},$$  

$$\Phi(h) = \sum_{m=1}^s \gamma_m (\phi_m^+(h/m) + \phi_m^-(h/m)) \quad \text{(symmetric)}.$$

We will show below that under appropriated hypothesis, the integrators given by (3a) and (3b) are convergent with order $q$, if $\gamma = (\gamma_1, \ldots, \gamma_s)$
verifies the following conditions

\begin{align}
1 &= \gamma_1 + \gamma_2 + \cdots + \gamma_s, \\
0 &= \gamma_1 + 2^{-k} \gamma_2 + \cdots + s^{-k} \gamma_s, \quad 1 \leq k \leq q - 1, \\
\frac{1}{2} &= \gamma_1 + \gamma_2 + \cdots + \gamma_s, \\
0 &= \gamma_1 + 2^{-2k} \gamma_2 + \cdots + s^{-2k} \gamma_s, \quad 1 \leq k \leq n - 1, 
\end{align}

respectively, where $2n = q$.

The number of steps of the methods (3) is bigger than the corresponding symplectic methods. Nevertheless, the possibility of computing $\phi_m^\pm$ simultaneously, allows to reduce significantly the total time of computation using multiple processors. The total number of step for (3a) is given by $S_T = 2 \sum_{m \neq 0}^\gamma m$ and $S_T = 4 \sum_{m \neq 0}^\gamma m$ for (3b).

Neglecting the communication time between the processors, the total time of computation working in parallel, turns out to be proportional to $S_P = 2 \max_{m \neq 0}^\gamma m$ in both cases. The system (4a) has solution for $s \geq q$, and hence there exist methods of arbitrary order $q$ with $S_P = 2q$ and $S_T = q(q + 1)$. On the other side, the system (4b) has solution for $s \geq n$, which shows that there exist integrators of arbitrary even order $q = 2n$ with $S_P = q$ and $S_T = q(q/2 + 1)$, using the double of processors. As it can be seen the minimum number of steps working in parallel for the symmetric method is smaller than the corresponding one for the asymmetric method. Also, in the examples considered, the symmetric method presents less error than the asymmetric method. These two latter issues pointed out justify the choice of the symmetric method over the asymmetric one. Let us mention that, in the examples developed in section 4 the implementation was done with a single processor.

The paper is organized as follows: In section 2 we give the basic definitions and preliminary results. Some elementary proofs were omitted. We define the stability and uniformly stability bounds for an application which extend the logarithmic norm notion given in [6]. Following the ideas of [3] and [7] we consider a decreasing sequence of dense subspaces where the flows are repeatedly differentiable. In section 3 we prove consistency and stability results for the methods (3), from where we deduce the convergence in the standard way. In section 4 we give several examples of the application of the methods to initial value problems for ODE’s and irreversible PDE’s. Also, we analyze a Hamiltonian equation and compare the results obtained for the methods presented...
in this paper with the ones for symplectic operators. Finally, in section 5 we present some conclusions and future work.

2. Notation and preliminary results

2.1. Combinatorial results. For $\beta = (\beta_1, \ldots, \beta_r) \in \mathbb{N}^r$ a multi-index, we define $\beta! = \beta_1! \cdots \beta_r!$. If $I_{r,k} = \{ \beta \in \mathbb{N}^r : \beta_1 + \cdots + \beta_r = k \}$, it verifies $\mathbb{N}^r = \bigcup_{k=0}^{\infty} I_{r,k}$.

Remark 2.1. It holds $I_{r,k} = \emptyset$ if $r > k$, $I_{k,k} = \{(1, \ldots, 1)\}$ and for $r + s \leq k$, $I_{r+s,k} = \bigcup_{j=s}^{k-r} I_{r,k-j} \times I_{s,j}$.

We will need the following lemmas. We skip the proofs since they are straightforward computations.

Lemma 2.1. If $\gamma$ verifies the conditions (4a), then for $1 \leq k \leq q$, it satisfies
\[
\sum_{m=r}^{s} \binom{m}{r} m^{-k} \gamma_m = 0, \quad r = 1, \ldots, k - 1,
\]
\[
\sum_{m=k}^{s} \binom{m}{k} m^{-k} \gamma_m = \frac{1}{k!}.
\]

Lemma 2.2. If $\gamma$ verifies the conditions (4b), then for $1 \leq k \leq q = 2n$, it satisfies
\[
\sum_{m=1}^{s} \left[ \binom{m}{r} + (-1)^{k+r} \binom{m}{r} \right] m^{-k} \gamma_m = 0, \quad r = 1, \ldots, k - 1,
\]
\[
\sum_{m=1}^{s} \left[ \binom{m}{k} + \binom{m}{k} \right] m^{-k} \gamma_m = \frac{1}{k!},
\]
where $\binom{m}{r} = \binom{m+r-1}{m-1}$.

2.2. Stable maps. Let $H$ be an Hilbert space, and $\varphi : \mathbb{R}_+ \times H \to H$ a continuous map such that $\varphi(h) = \varphi(h,.) : H \to H$ is Lipschitz continuous and $\varphi(0) = I$, we define
\[
\Lambda(\varphi, h) = \sup_{u, u' \in H, u \neq u'} \frac{\|\varphi(h, u) - \varphi(h, u')\|}{\|u - u'\|}.
\]

We will say $\varphi$ is stable iff $\kappa(\varphi) = \limsup_{h \downarrow 0} h^{-1}(\Lambda(\varphi, h) - 1) < \infty$. For any $\kappa > \kappa(\varphi)$, there exists $h_* = h_*(\kappa)$ such that
\[
\Lambda(\varphi, h) \leq 1 + \kappa h \leq e^{\kappa h}.
\]
if $0 < h < h_s$. For $\varphi$ a linear flow, $\kappa(\varphi)$ is the logarithmic norm of the generator (see [6]). A map $\varphi$ is uniformly stable iff

$$
\mu(\varphi) = \limsup_{h \downarrow 0} h^{-1} \Lambda(\varphi - I, h) < \infty,
$$

since $\Lambda(\varphi, h) \leq 1 + \Lambda(\varphi - I, h)$, uniformly stable implies stable. Observe that the family of (uniformly) stable maps is scale-invariant and if $\varphi_\lambda(h, u) = \varphi(\lambda h, u)$ with $\lambda > 0$, then $\kappa(\varphi_\lambda) = \lambda \kappa(\varphi)$, $\mu(\varphi_\lambda) = \lambda \mu(\varphi)$. If $\varphi$ is a strongly continuous semi-group, $\varphi$ is stable but it is uniformly stable if and only if the infinitesimal generator is a bounded operator.

**Proposition 2.1.** If $\phi_0, \phi_1$ are (uniformly) stable, then the map $\varphi$ defined by $\varphi(h, u) = \phi_0(h, \phi_1(h, u))$, is (uniformly) stable and $\kappa(\varphi) \leq \kappa(\phi_0) + \kappa(\phi_1)$ ($\mu(\varphi) \leq \mu(\phi_0) + \mu(\phi_1)$).

**Proof.** Since $\Lambda(\varphi, h) \leq \Lambda(\phi_0, h)\Lambda(\phi_1, h)$, it holds

$$
\frac{\Lambda(\varphi, h) - 1}{h} \leq \frac{\Lambda(\phi_0, h) - 1}{h} \Lambda(\phi_1, h) - 1 + \frac{\Lambda(\phi_0, h) - 1}{h},
$$

using $\Lambda(\phi_0, h) \rightarrow 1$, we get the stability. Writing $\varphi - I = (\phi_0 - I) \circ \phi_1 + \phi_1 - I$, we have

$$
\Lambda(\varphi - I, h) \leq \Lambda(\phi_0 - I, h)\Lambda(\phi_1, h) + \Lambda(\phi_1 - I, h),
$$

and then $\mu(\varphi) \leq \mu(\phi_0) + \mu(\phi_1)$.

Let $\{\phi_m\}_{1 \leq m \leq s}$ be stable maps and $\Phi$ an affine combination, i.e. $\Phi = \gamma_1 \phi_1 + \cdots + \gamma_s \phi_s$ with $\gamma_1 + \cdots + \gamma_s = 1$, it is easy to see that

$$
\Lambda(\Phi, h) \leq \sum_{m=1}^s |\gamma_m| \Lambda(\phi_m, h),
$$

therefore, $\Phi$ is not necessarily a stable map (but it is true for convex combinations). We have

**Proposition 2.2.** If $\{\phi_m\}_{1 \leq m \leq s}$ are uniformly stable maps, then an affine combination $\Phi$ is uniformly stable.

**Proof.** Writing $I = \gamma_1 I + \cdots + \gamma_s I$ and $\Phi - I = \gamma_1 (\phi_1 - I) + \cdots + \gamma_s (\phi_s - I)$, we get $\mu(\Phi) \leq \sum_{1 \leq m \leq s} |\gamma_m| \mu(\phi_m)$.

2.3. Compatible flows. Let $\{H_k\}_{k \geq 0}$ be Hilbert spaces verifying $H_{k+1} \hookrightarrow H_k$, we define for $k \geq 0$

$$
D_k = \{ f \in C^\infty(H_k, H_0) : f|_{H_{k+1}} \in C^\infty(H_{k+1}, H_l) \text{ for all } l \geq 0 \},
$$

we can see that if $f \in D_k$ and $g \in D_j$, then $f \circ g \in D_{j+k}$. We will say $\varphi \in C([0, h_s] \times H, H)$ is compatible with $\{H_k\}_{k \geq 0}$ iff $\varphi \in C^{k, \infty}([0, h_s] \times H_{k+l}, H_l)$, for all $l \geq 0$. As an example, let $A : D(A) \to H$ be a
Proof. The proof is by induction, suppose the result holds for $1 \leq j \leq k - 1$, using the lemma above we obtain

$$L_k[\varphi \circ \varphi] = 2L_k[\varphi] + \sum_{j=1}^{k-1} \binom{k}{j} L_{k-j}[\varphi] L_{j}[\varphi]$$

$$= 2L_k[\varphi] + \sum_{j=1}^{k-1} \binom{k}{j} L_1[\varphi]^{k-j} L_1[\varphi]^j = 2L_k[\varphi] + (2^k - 2)L_1[\varphi]^k.$$
Since \( \varphi(h) \circ \varphi(h) = \varphi(2h) \), it is verified
\( L_k[\varphi \circ \varphi] = 2^k L_k[\varphi] \), which implies the result for \( k \).

\[ \square \]

### 3. Convergence

3.1. **Consistency.** In order to get consistency results for the schemes given by (3a) and (3b), the coefficients of an affine combination have to verify the algebraic conditions (4a) and (4b), respectively. We will make the following assumptions: the flow \( \varphi \) associated to (1) and the partial flows \( \varphi_0 \) and \( \varphi_1 \) are compatible with \( \{ H_k \}_{k \geq 0} \). We have the following consistency results:

**Theorem 3.1** (Asymmetric case). If \( \gamma \) verifies (4a), for any \( u \in H_q \) the method \( \Phi \) given by (3a) satisfies

\[
\frac{\partial^k \Phi}{\partial h^k}(0, u) = \frac{\partial^k \varphi}{\partial h^k}(0, u),
\]

for \( k = 0, \ldots, q \).

**Theorem 3.2** (Symmetric case). If \( \gamma \) verifies (4b), for any \( u \in H_q \) the method \( \Phi \) given by (3b) satisfies

\[
\frac{\partial^k \Phi}{\partial h^k}(0, u) = \frac{\partial^k \varphi}{\partial h^k}(0, u),
\]

for \( k = 0, \ldots, q \).

3.1.1. **Asymmetric case.** We prove the consistency of method (3a) using lemma 2.3 and lemma 2.1.

**Proposition 3.1.** Let \( \varphi \in C([0, h] \times H, H) \) be a compatible map with \( \{ H_k \}_{k \geq 0} \) verifying \( \varphi(0) = I \). Let \( \varphi_1 = \varphi \) and \( \varphi_{m+1} = \varphi \circ \varphi_m \), then

\[
L_k[\varphi_m] = \sum_{r=1}^{k} \binom{m}{r} \sum_{\beta \in I_{r,k}} \frac{k!}{\beta!} L_{\beta_1}[\varphi] \ldots L_{\beta_r}[\varphi].
\]

**Proof.** Using lemma 2.3 we get

\[
L_k[\varphi_{m+1}] = L_k[\varphi_m] + L_k[\varphi] + \sum_{j=1}^{k-1} \binom{k}{j} L_{k-j}[\varphi_m] L_j[\varphi],
\]

applying induction and using remark 2.1 we obtain the result. \( \square \)

**Proposition 3.2.** If \( \gamma \) verifies (4a), the method \( \Phi \) given by (3a) satisfies

\[
L_k[\Phi] I = L_1[\varphi]^k I, \text{ for } k = 1, \ldots, q.
\]
Proof. Since \( L_k[\Phi]I = \sum_{r=1}^{s} m^{-1} \gamma_{m} L_k[\varphi_m]I \), using proposition 3.1 we can see
\[
L_k[\Phi]I = \sum_{r=1}^{s} \left( \sum_{m=1}^{s} \left( \sum_{r=1}^{s} m^{-1} \gamma_{m} \right) \right) \sum_{\beta \in I_{r,k}} \frac{k!}{\beta!} L_{\beta_1}[\varphi] \ldots L_{\beta_r}[\varphi]I,
\]
from lemma 2.1 we get \( L_k[\Phi]I = \sum_{\beta \in I_{k,k}} \frac{k!}{\beta!} L_{\beta_1}[\varphi] \ldots L_{\beta_r}[\varphi]I = L_1[\varphi]^k I \).

Proof. (Theorem 3.1) Since \( \phi^+ = \phi_1 \circ \phi_0 \), it holds \( L_1[\phi^+] = L_1[\phi_0] + L_1[\phi_1] = L_1[\phi] \). Using proposition 3.2 we obtain
\[
\frac{\partial^k \phi}{\partial h^k}(0, u) = (L_1[\phi^+]kI)(u) = (L_1[\phi]kI)(u)
\]
and the theorem follows.

3.1.2. Symmetric case. If \( \phi_0, \phi_1 \) were reversible flows, then it would hold \( \phi^-(h) \circ \phi^+(-h) = I \) and using lemma 2.3, \( M_k = 0 \), where \( M_k \) is defined by (5). We get the same result for irreversible flows:

Lemma 3.1. Let \( M_k : \mathcal{D}_0 \to \mathcal{D}_k \) be the operator given by
\[
(5) \quad M_k = \sum_{j=0}^{k} (-1)^j \binom{k}{j} L_j[\phi^+]L_{k-j}[\phi^-],
\]
then \( M_k = 0 \).

Proof. Using lemma 2.3 for \( \phi^\pm \) and lemma 2.4, we can write \( M_k \) as
\[
M_k = \sum_{j=0}^{k} \sum_{i=0}^{j} \sum_{l=0}^{j-i} (-1)^j \binom{k}{j} \binom{j}{i} \binom{j-i}{l} L_1[\phi_0]^{j-i} L_1[\phi_1]^{k+i-j-l} L_1[\phi_0]^l.
\]
Interchanging the order of summation, considering \( n = j - i \) and using
\[
\binom{k}{n+i} \binom{n+i}{i} \binom{k-n-i}{l} = \binom{k-n-l}{i} \frac{k!}{n!(k-n-l)!},
\]
we can write \( M_k \) as
\[
M_k = \sum_{n=0}^{k} (-1)^n \sum_{l=0}^{k-n-1} \left( \sum_{i=0}^{k-n-l} (-1)^i \binom{k-n-l}{i} \right) \frac{k!}{n!(k-n-l)!} \times
\]
\[
x L_1[\phi_0]^n L_1[\phi_1]^{k-n-l} L_1[\phi_0]^l + \sum_{n=0}^{k} (-1)^n \binom{k}{k-n} L_1[\phi_0]^k.
\]
Since \( \sum_{i=0}^{k-n-l} (-1)^i \binom{k-n-l}{i} = 0 \), we have the result.
Proposition 3.3. For \( m \geq 1 \) it holds

\[
L_k[\phi_m^-] = (-1)^k \sum_{r=1}^{k} C_{m,r} \sum_{\beta \in I_{r,k}} \binom{k!}{\beta} \beta! \sum_{\gamma \in I_{r,k}} \beta \gamma \phi_{\gamma}^+ \cdots \phi_{\beta}^+,
\]

where \( C_{m,r} = (-1)^r \left( \binom{m}{r} \right) = (-1)^r \left( \frac{m + r - 1}{r} \right) \).

Proof. We proceed by induction: eliminating \( L_k[\phi^-] \) from (5) and using similar arguments as proposition 3.1 we obtain the case \( m = 1 \). Applying lemma 2.3 to \( \phi_m^- = \phi \circ \phi_m^- \) and using \( C_{m+1,r} = \sum_{s=0}^{r} C_{m,s} C_{1,r-s} \), we have the result.

Proposition 3.4. If \( \gamma \) verifies conditions (1b), then method \( \Phi \) defined by (3b) satisfies \( L_k[\Phi] I = (L_k[\phi^+])^k I \) for \( k = 0, \ldots, 2n \).

Proof. Applying proposition 3.1 to \( \phi^+ \), using proposition 3.3 and lemma 2.2 we obtain the result.

Proof. (theorem 3.2) From proposition 3.4 we have

\[
\frac{\partial^k \Phi}{\partial h^k}(0, u) = (L_1[\phi^+]^k I)(u) = (L_1[\phi] I)(u),
\]

and the theorem follows.

3.2. Stability. If \( A_0 \) and \( A_1 \) are continuous Lipschitz maps, from Duhamel integral and Gronwall inequality, we have maps \( \phi_0, \phi_1 \) and then \( \Phi \) are uniformly stable. Except for ordinary differential equations, this is not the case. However, if \( A = A_0 + A_1 \), where \( A_0 \) is the infinitesimal generator of strongly continuous semi-group and \( A_1 \) is a local Lipschitz continuous map, we show the methods are stable.

Proposition 3.5. Let \( \phi_0 \) a strongly continuous semi-group such that

\[
\|\phi_0(h, u)\|_H \leq e^{\kappa_0 h} \|u\|_H
\]

and \( \phi_1 \) a uniformly stable map, then \( \Phi \) is a stable map.

Proof. Using \( \phi_0 = 2 \sum_{m=1}^{s} \gamma_m \phi_0 \), we see that \( \Phi = \phi_0 + \sum_{m=1}^{s} \gamma_m (\psi_m^+ + \psi_m^-) \), where \( \psi_m^+(h) = \phi_m^+(h/m) - \phi_0(h) \). Thus, we have

\[
\Lambda(\Phi, h) - 1 \leq \Lambda(\phi_0, h) - 1 + \sum_{m=1}^{s} |\gamma_m| (\Lambda(\psi_m^+, h) + \Lambda(\psi_m^-, h)).
\]

We use an inductive argument to show

\[
\limsup_{h \downarrow 0} h^{-1} \Lambda(\psi_m^\pm, h) \leq \mu(\phi_1).
\]

For \( m = 1 \), we have

\[
\psi_1^+(h) = (\phi_1(h) - I) \circ \phi_0(h), \quad \psi_1^-(h) = \phi_0(h) \circ (\phi_1(h) - I),
\]
since \( \Lambda(\psi^\pm_1, h) \leq \Lambda(\phi_0 - I, h) \Lambda(\phi_0, h) \) and \( \lim_{h \downarrow 0} \Lambda(\phi_0, h) = 1 \), it verifies
\[
\limsup_{h \downarrow 0} h^{-1} \Lambda(\psi^\pm_m, h) \leq \mu(\phi_1).
\]
For \( m > 1 \), it holds
\[
\psi^\pm_m(h) = \psi^\pm_1(h/m) \circ \phi^\pm_{m-1}(h/m) + \phi_0(h/m) \circ \psi^\pm_{m-1}((m-1)h/m),
\]

hence
\[
\Lambda(\psi^\pm_m, h) \leq \Lambda(\psi^\pm_1, h/m) \Lambda(\phi^\pm_{m-1}, h/m) + \Lambda(\phi_0, h/m) \Lambda(\psi^\pm_{m-1}, (m-1)h/m).
\]
By inductive hypothesis and \( \lim_{h \to 0} \Lambda(\phi^\pm_{m-1}, h) = 1 \), we obtain (6) and therefore \( \kappa(\Phi) \leq c_0 + 2 \sum_{m=1}^s \gamma_m \mu(\phi_1) \).

3.3. Convergence results. We assume \( \phi, \phi_0, \phi_1 \) are compatible with \( \{H_k\}_{k \geq 0} \), a sequence of Hilbert spaces with \( H_0 = \mathcal{H} \) and \( H_{k+1} \hookrightarrow H_k \).

We suppose that for any \( R > 0 \), there exists \( T = T(R) > 0 \) such that if \( u_0 \in B(H, 0, R) \), then \( \phi(t, u_0) \), \( \phi(t, u_0) \) and \( \phi_1(t, u_0) \) are defined on \( [0,T] \), and if \( u_0 \in H_k \), the solution in \( H_k \) last as long as in \( \mathcal{H} \). We require \( \phi_0, \phi_1 \) verify the hypothesis of proposition 3.5 on \( B(H, 0, R) \).

Hence, by decreasing \( T \) if necessary, \( \phi^\pm_{m}(t, u_0) \) and \( \Phi(t, u_0) \) are defined on \( [0,T] \). We have the following convergence result

**Theorem 3.3.** Let \( u_0 \in H_{q+1} \) and \( u(t) = \phi(t, u_0) \) the maximal solution of (1) defined on \( [0,T_*] \). For any \( T \in (0,T_*), \) there exists \( h_*, \delta, M, \kappa > 0 \) such that if \( U_0 \in H_{q+1} \) verifies \( \|u_0 - U_0\|_{\mathcal{H}} < \delta \) and \( 0 < h < h_* \), then the sequence \( U_T = \Phi(h, U_{T-1}) \) is defined for \( \tau \leq T/h \) and verifies
\[
\|u_\tau - U_\tau\|_{\mathcal{H}} \leq e^{\kappa \tau h} \|u_0 - U_0\|_{\mathcal{H}} + M e^{\kappa \tau h} - \frac{1}{\kappa} h^q.
\]

where \( u_\tau = u(\tau h) \).

**Remark 3.1.** These conditions may seem too restrictive, nevertheless they are verified in many evolution problems. As an example, we consider the NLS equation with \( \mathcal{H} = H^s(\mathbb{R}^d) \) the Sobolev spaces consisting of the \( \sigma \) times derivable functions and \( H_k = H^{s+2k}(\mathbb{R}^d) \). Clearly, the unitary group generated by \( i \nabla^2 \) is compatible with \( \{H_k\}_{k \geq 0} \). It is known that if \( \sigma > d/2 \), the spaces \( H_k \) are Banach algebras with the punctual product of functions, therefore any application as \( A_1(u) = P(u, u^*) \), where \( P \) is a polynomial such that \( P(0,0) = 0 \), turns out to be locally Lipschitz in \( H_k \), implying the existence of the flow \( \phi_1 \). Being \( A_1 \) a polynomial application, is infinitely derivable and its derivatives are locally Lipschitz, proving that the flow \( \phi_1 \) is compatible with \( \{H_k\}_{k \geq 0} \). From the following estimate
\[
\|A_1(u)\|_{H_k} \leq C(\|u\|_{H_k})\|u\|_{H_k},
\]
we deduce that the times of existence of the solutions do not depend on $k$. We refer to [4] for the proof of the mentioned properties of the flow $\phi$ associated to the NLS initial value problem.

Proof. The proof is by induction on $\tau$. Let $R = 2 \max_{t \in [0,T]} \|u(t)\|_H$, $\kappa = \kappa_R(\Phi)$ and

$$ M = \frac{1}{(q + 1)!} \max_{(t,u) \in K} \left\| \frac{\partial^{q+1} \phi}{\partial t^{q+1}}(t,u) \right\|_H + \left\| \frac{\partial^{q+1} \Phi}{\partial t^{q+1}}(t,u) \right\|_H, $$

where $K$ is the compact set of $\mathbb{R}^+ \times H_{q+1}$ given by $K = [0,T] \times \{u(t)\}_{t \in [0,T]}$, taking $\delta > 0$ and $0 < h_* < T(R)$ such that

$$ e^{\kappa T} \delta + M e^{\kappa T} - \frac{1}{\kappa} h_*^q < R/2, $$

using inductive hypothesis, we obtain

$$ \|U_{\tau-1}\|_H \leq \|u_{\tau-1}\|_H + \|U_{\tau-1} - u_{\tau-1}\|_H \\ \leq R/2 + e^{\kappa(\tau-1)h} \|u_0 - U_0\|_H + M e^{\kappa(\tau-1)h} - \frac{1}{\kappa} h^q \\ \leq R/2 + e^{\kappa T} \delta + M e^{\kappa T} - \frac{1}{\kappa} h_*^q < R, $$

hence

$$ \|\Phi(h,u_{\tau-1}) - \Phi(h,U_{\tau-1})\|_H \leq e^{\kappa h} \|u_{\tau-1} - U_{\tau-1}\|_H. $$

Let $\theta \in C^{q+1}([0,h],H)$ given by $\theta(t) = \phi(t,u_{\tau-1}) - \Phi(t,u_{\tau-1})$, from theorem [3.2] we get $\theta^{(k)}(0) = 0$, for $0 \leq k \leq q$, using (7), we see

$$ \|\theta^{(q+1)}(h)\|_H \leq M h^{q+1}. $$

From estimates (8) y (9), we get $\|u_{\tau} - U_{\tau}\|_H \leq e^{\kappa h} \|u_{\tau-1} - U_{\tau-1}\|_H + M h^{q+1}$. Using $e^{\kappa h} \geq 1 + \kappa h$, the result follows.

The computation of $\Phi$ requires to solve exactly the partial problems. Besides some simple cases of ordinary differential equations, this is not possible. In what follows we will show that we can define integration methods of order $q$ using suitable approximations of the flows $\phi_0$ y $\phi_1$. Let $\Psi \in C([0,h_*) \times H,H)$ verifying

$$ \|\Psi(h,u) - \Phi(h,u)\|_H \leq \rho $$

for $u \in B_H(R,0)$. Let $V_0 = U_0$ and $V_{\tau} = \Psi(h,V_{\tau-1})$, from the stability of $\Phi$ we get that

$$ \|U_{\tau} - V_{\tau}\|_H \leq C e^{\kappa h} - \frac{1}{e^{\kappa h} - 1} \rho. $$
Let $\psi_j$ be an approximation of $\phi_j$ such that $\|\phi_j(h,u) - \psi_j(h,u)\|_H \leq Ch^{q+1}$, $j = 0, 1$. Then the application $\Psi$ defined by (3) with $\psi_j$ in place of $\phi_j$ verifies the condition (10) with $\rho = Ch^{q+1}$ and consequently the method $\Psi$ satisfies

$$\|u_\tau - V_\tau\|_H \leq e^{\kappa \tau h} \|u_0 - V_0\|_H + M \frac{e^{\kappa \tau h} - 1}{\kappa} h^q.$$  

We consider the following example. Let $\{u_n\}_{n \in \mathbb{N}}$ be an orthonormal basis of $H$ and $\phi_0(t,u) = \sum_{n \in \mathbb{N}} e^{\alpha_n t} \langle u_n, u \rangle u_n$ with $\Re \alpha_n \leq \kappa$. We define the spaces

$$H_k = \{ u \in H : \sum_{n \in \mathbb{N}} |\alpha_n|^{2k} |\langle u_n, u \rangle|^2 < \infty \},$$

so that $\phi_0$ becomes compatible with $\{H_k\}_{k \geq 0}$ and verifies $\|\phi_0(t,u)\|_{H_k} \leq e^{\kappa t} \|u\|_{H_k}$. If we take $\psi_0(t,u) = \sum_{1 \leq n \leq N} e^{\alpha_n t} \langle u_n, u \rangle u_n$, we obtain that

$$\|\phi_0(h,u) - \psi_0(h,u)\|_H \leq e^{\kappa h} \inf_{n > N} |\alpha_n|^{-k} \|u\|_{H_k}.$$  

Hence, if $\lim \inf_{n \to \infty} |\alpha_n| = +\infty$, for $h > 0$, there exists a $N = N(h)$ large enough such that $\|\phi_0(h,u) - \psi_0(h,u)\|_H \leq Ch^{q+1}$.

4. Numerical examples

We present several examples which illustrate the performance of the proposed methods.

4.1. Ordinary differential system. We first consider an elementary ordinary differential system, which is very simple to approach with the methods described in the previous sections but it would be more costly to solve with symplectic methods, since in this case the time steps should be very small to be able to go backwards. The bidimensional system

$$(11) \begin{cases} \dot{u}_1 = 4u_2 - \tan(u_1), \\ \dot{u}_2 = -4u_1 - \tan(u_2), \end{cases}$$

can be split, in a natural way, into a linear problem and decoupled equations. The flow is a clockwise rotation and there orbits are indicated by circles in figure 1. The paths converging to the origin represents the trajectories of the equations $\dot{u}_j = -\tan(u_j)$ which solutions are $u_j(t) = \arcsin(e^{-t} \sin(u_{j,0})$, for $j = 0, 1$. Observe that the solution is not defined for $t < \ln |\sin(u_{j,0})| \leq 0$, what delimits the value of $h$ for symplectic operators. In the same figure we show the exact solution (with Runge–Kutta for very small step) with initial datum $(1, 3/2)$ for $t \in [0, 2]$ and the dots representing the values obtained with our method $\Phi$ of order 4 with step $h = 0.2$. We note that the symplectic
operator of order 4 proposed in [11] (and in [15]) is not defined for that value of $h$. To apply this method it is necessary to reduce significantly the step $h$.

4.2. Oscillatory reaction–diffusion system. In this example, we study the behaviour of the methods of a reaction–diffusion system, as the ones shown in [8], we consider the system

\begin{align}
  v_t &= \nabla^2 v + (1 - r^2)v - (\omega_0 - \omega_1 r^2)v,
  \\
  w_t &= \nabla^2 w + (\omega_0 - \omega_1 r^2)v + (1 - r^2)w,
\end{align}

where $r^2 = v^2 + w^2$. If $u = v + iw$, equation (12) reads as follows:

\begin{align}
  u_t &= \nabla^2 u + (1 - |u|^2)u + i(\omega_0 - \omega_1 |u|^2)u.
\end{align}

The right hand member can be splitted and rewritten as $A_0 u + A_1(u)$, where $A_0(u) = \nabla^2 u$ and

\begin{align}
  A_1(u) &= (1 - |u|^2)u + i(\omega_0 - \omega_1 |u|^2)u.
\end{align}

The flow $\phi_1$ is given by

\begin{align}
  \phi_1(h, u_0) &= u_0 e^{h(1 + (e^{2h} - 1)|u_0|^2)^{-1/2}} e^{i(\omega_0 h - \omega_1 / 2 \ln(1 + (e^{2h} - 1)|u_0|^2))}.
\end{align}
We will restrict our discussion to \( L \)-periodic solutions, flow \( \phi_0 \) can be computed approximately by using discrete Fourier transform (DFT). Let \( \eta \) be an odd integer, \( \eta = 2l + 1 \), consider

\[
(I_{\eta}u)(x) = \sum_{s=-l}^{l} \hat{U}_se^{iasx},
\]

where \( a = 2\pi/L, \hat{U}_s \) is DFT coefficient given by

\[
\hat{U}_s = \frac{1}{\eta} \sum_{r=0}^{\eta-1} U_re^{-i2\pi rs/\eta} = \frac{1}{\eta} \sum_{r=0}^{\eta-1} u(Lr/\eta)e^{-i2\pi rs/\eta}.
\]

Since \( e^{-i2\pi rs/\eta} = e^{-i2\pi r(s+\eta)/\eta} \), it holds \( \hat{U}_s = \hat{U}_{s+\eta} \). In [14] (lemma 2.2) it is shown

\[
\|u - I_{\eta}u\|_{L^2(\mathbb{T})} \leq C_{L,\sigma} \eta^{-\sigma}\|u\|_{H^\sigma(\mathbb{T})},
\]

for \( \sigma > 1/2 \), thus

**Proposition 4.1.** If \( \psi_0(h) = \phi_0(h)I_{\eta} \), for \( u \in H^\sigma(\mathbb{T}) \), it holds

\[
\|\psi_0(h)u - \phi_0(h)u\|_{L^2(\mathbb{T})} \leq C_{L,\sigma} \eta^{-\sigma}\|u\|_{H^\sigma(\mathbb{T})}.
\]

From the definition of \( \psi_0(h) \) and \( \hat{U}_s = \hat{U}_{s+\eta} \), we get

\[
(\psi_0(h)u)(Lr/\eta) = \sum_{s=-l}^{l} \hat{U}_se^{-a^2s^2t}e^{i2\pi rs/\eta} = \sum_{s=l+1}^{\eta-1} \hat{U}_se^{-a^2(\eta-s)^2t}e^{i2\pi rs/\eta}
\]

\[
+ \sum_{s=0}^{l} \hat{U}_se^{-a^2s^2t}e^{i2\pi rs/\eta} = \sum_{s=0}^{\eta-1} \hat{U}_se^{-a^2\lambda_st}e^{i2\pi rs/\eta},
\]

where \( \lambda_s = \eta^2g(s/\eta) \) for \( 0 \leq s \leq \eta - 1 \) and \( g(\xi) = \xi^2 - 2(\xi - 1/2)^2 \).

In [8], it is proven stability of plane waves

\[
v(x, t) = r^*\cos(\theta_0 \pm ax + (\omega_0 - \omega_1 r^*t)t),
\]

\[
w(x, t) = r^*\sin(\theta_0 \pm ax + (\omega_0 - \omega_1 r^*t)t),
\]

if \( L > 2\pi(3 + 2\omega_1^2)^{1/2} \), where \( r^* = L^{-1}(L^2 - 4\pi^2)^{1/2} \) (see [13]). Taking \( L = 4\pi, \omega_0 = 1, \omega_1 = 1/2 \) and \( u_0 = r^*e^{iax} \), in figure 2 we compare global errors for \( T = 10 \) for methods given by [35] of order \( q = 4, 6, 8 \) with \( \eta = 63 \). We note that the slopes coincide with the expected order up to the point where the rounding error dominates the total error.

In order to show the stability of plane waves, in figure 3 we consider \( \tilde{u}_0(x) = 0.8u_0(x) + 0.1 + 2.5e^{2ax} - 0.8ie^{3ax} \) and plot in solid line \( \Phi(t, \tilde{u}_0) \) and in dotted line \( \phi(t, u_0) \) for \( t = 0 \) and \( t = 50 \), \( \eta = 63 \) and \( h = 0.1 \).
4.3. Logarithmic Gross–Pitaevskii equation. In order to compare with symplectic integrators, we consider a Hamiltonian problem. In [10], it is considered the equation

\[ i\hbar \psi_t = -\frac{\hbar^2}{2m} \psi_{xx} + \frac{1}{2} m \omega^2(t) x^2 \psi - F(t) x \psi - \frac{\hbar \lambda}{2} \ln |\psi|^2 \psi. \]

If \( F(t) \equiv 0 \) and \( \omega(t) \equiv \omega_0 \) and taking the new variables

\[ x \to x/\sqrt{m\omega_0/\hbar}, \quad t \to t/\omega_0, \]

we obtain

\[ iu_t = -\frac{1}{2} u_{xx} + \frac{1}{2} x^2 u - \alpha \ln |u|^2 u. \]

with \( \alpha = \lambda/(2\omega_0) \). There are solutions of (13) of the form \( u(x, t) = e^{-\beta(it+x^2)} \), with \( \beta = (\alpha + \sqrt{\alpha^2 + 1})/2 \). Using similar arguments as for logarithmic Schrödinger equation (see [5] and [4] sections 9.2–9.3) one
can show that problem (13) is well-posed. The linear problem
\[
\begin{align*}
{i}u_t &= -\frac{1}{2}u_{xx} + \frac{1}{2}x^2 u, \\
   u(0) &= u_0.
\end{align*}
\]

can be solved explicitely using the expansion base on the eigenfunctions of the operator given by
\[
h_s(x) = \pi^{-1/4}(2^s s!)^{-1/2} H_s(x)e^{-\frac{1}{2}x^2}
\]
with eigenvalues \(\mu_s = s + 1/2\), where \(H_s(x)\) are the usual Hermite polynomials. Thus, the solution is given by \(u(x,t) = \sum_{s \geq 0} \langle h_s, u_0 \rangle e^{-i\mu_s t} h_s(x)\).

The nonlinear problem \(i u_t = -\alpha \ln |u|^2 u\) has solution \(u(x,t) = e^{i\alpha \ln |u_0(x)|^2 t} u_0(x)\). In [2], the Fourier–Hermite coefficients are calculated by Gauss–Hermite quadrature, i.e.
\[
(\psi_0(h)u)(x_r) = \sum_{s=0}^{n-1} \hat{U}_s e^{-i\mu_s h} h_s(x_r),
\]
where \(\hat{U}_s = \sum_{r=0}^{n-1} w_r h_s(x_r) u(x_r)\), with \(x_r\) the roots of the \(H_\eta(z)\), and the associated weights \(w_r\) given by \(w_r = \eta^{-1} h^{-2} \eta^{-1}(x_r)\) (see [7] for error estimates). If we define matrix \([\Omega]_{s,r} = w_s \delta_{s,r}\), \([G]_{s,r} = h_s(x_r)\) and \([M]_{s,r} = \mu_r \delta_{s,r}\), we have \(\psi_0(h) = G^T e^{-i M} G \Omega\).

Let \(\alpha = 3/4\), for initial data \(u_0(x) = e^{-x^2}\) the solution is \(u(x,t) = e^{-it} u_0(x)\), which is the ground state of the Hamiltonian
\[
\mathcal{H}(u) = \frac{1}{4} \int_{\mathbb{R}} (|u_x|^2 + x^2 |u|^2 - 2 \alpha \ln |u|^2 |u|^2) \, dx,
\]
subject to \(Q(u) = \|u\|_{L^2}^2 = \sqrt{\pi}/2\), the value of the energy is \(\mathcal{H}(u_0) = \sqrt{\pi}/8\). In figure [4], we plot global error vs. \(h\) for \(t \in [0, 2]\), in solid line we show the error for \(\Phi\) and in dashed line for \(\Phi_S\). We take \(\eta = 63\) and the norm
\[
\|u - U\| = \max_{0 \leq \tau \leq T/h} \left( \sum_{r=0}^{n-1} w_r |u(x_r, \tau h) - U_r(\tau h)|^2 \right)^{1/2}.
\]
The error for fourth order methods is shown in the left panel, in the right panel for sixth order. In figures [5] [6] it is shown the evolution of \(Q(u) - Q(u_0)\) and \(\mathcal{H}(u) - \mathcal{H}(u_0)\), with \(h = 0.01\), \(0 \leq \tau \leq 200\) (\(T = 2\)), for \(\Phi\) (solid line) and \(\Phi_S\) (dashed line).

We can see that the behaviour of the constants of the motion \(Q, \mathcal{H}\) for symplectic method of fourth order is better than for \(\Phi\) of the same order, but it is worse for sixth order.
Figure 4. Global error $\Phi$ vs $h$.

Figure 5. Evolution of $Q(u)$ for $\Phi_S y \Phi$ with $h = 0.01$.

Figure 6. Evolution of $H(u)$ for $\Phi_S y \Phi$ with $h = 0.01$.

5. Conclusions

Efficient methods for solution of large class of evolution problems was presented and the theoretical foundation was given. This was practically exemplified for a two-dimensional ODE system and a reaction-diffusion problem. A Hamiltonian problem was considered, in order to compare with symplectic methods. We note that these methods could be applied to the gradient descent method used to search minimum energy for a Hamiltonian (see [1] section 3), as we intend to do in a future work.

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