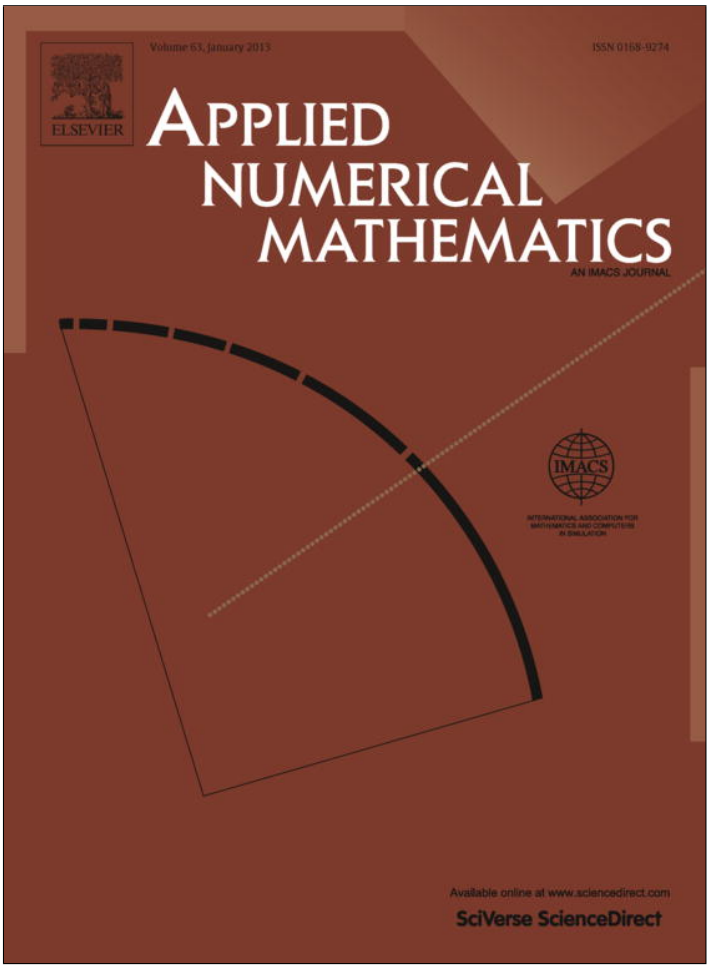

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Embedded exponential operator splitting methods for the time integration of nonlinear evolution equations

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ABSTRACT

In this work, we introduce embedded exponential operator splitting methods for the adaptive time integration of nonlinear evolution equations. In the spirit of embedded Runge–Kutta methods, such pairs of related higher-order split-step methods provide estimates of the local error with moderate additional computational effort as substeps of the basic integrator are reused to obtain a local error estimator.
As illustrations, we construct a split-step pair of orders 4(3) involving real method coefficients, tailored for nonlinear Schrödinger equations, and two order 4(3) split-step pairs with complex method coefficients, appropriate for nonlinear parabolic problems. Our theoretical investigations and numerical examples show that the splitting methods retain their orders of convergence when applied to evolution problems with sufficiently regular solutions. Furthermore, we demonstrate the ability of the new algorithms to serve as a reliable basis for error control in the time integration of nonlinear evolution equations by applying them to the solution of two model problems, the two-dimensional cubic Schrödinger equation with focusing singularity and a three-dimensional reaction–diffusion equation. Moreover, we demonstrate the advantages of our real embedded 4(3) pair of splitting methods over a pair of unrelated schemes for the time-dependent Gross–Pitaevskii equation.

1. Introduction

Over the years, it has become widely appreciated that adaptive time stepsize selection and error control based on reliable a posteriori estimates of the local error is the key to large scale computations of evolution equations. In previous decades, this understanding was still rather vague, see for instance [26, §15.2]:

> *A good ODE integrator should exert some adaptive control over its own progress, making frequent changes in its stepsize. Usually the purpose of this adaptive stepsize control is to achieve some predetermined accuracy in the solution with minimum computational effort. Many small steps should tiptoe through treacherous terrain, while a few great strides should speed through smooth uninteresting countryside. The resulting gains in efficiency are not mere tens of percents or factors of two; they can sometimes be factors of ten, a hundred, or more.*

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Recently, this intuitive understanding was also put on firm theoretical ground. In [19, Theorem 6] the efficiency of using an adaptive procedure as compared to the solution on a uniform time grid is specified quantitatively. The gain is shown to depend on the variation of the principal error function and is zero if the latter is a constant function on the interval of integration. Algorithms implementing successful time stepsize selection based on control theory and methods of signal processing are extensively discussed in [27–29], and even demonstrated to enhance computational stability. As the basis for any successful adaptive time stepsize selection, an estimate for the local error is needed.

In the present work, we are concerned with the reliable time integration of nonlinear evolution equations by higher-order exponential operator splitting methods [13,24] based on an adaptive time stepsize control. We employ a general framework of nonlinear evolution equations

$$u'(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big), \quad t_0 \leqslant t \leqslant T, \quad u(t_0) \text{ given}, \tag{1}$$

on a finite or infinite dimensional Banach space which allows to incorporate a wide scope of applications, see for instance [9,11,17,23,25]. Typically, problem (1) originates from an abstract formulation or spatial semi-discretisation of a partial differential equation subject to initial and boundary conditions. As model problems, we consider the two-dimensional cubic Schrödinger equation with focusing singularity, leading to a blowup-like behaviour and thus the need for an adaptive reduction of the time stepsizes when approaching the blowup time, a three-dimensional nonlinear reaction–diffusion equation, where the dissipativity of the problem allows to increase the time stepsizes adaptively, and the Gross–Pitaevskii equation modelling Bose–Einstein condensation. A fundamental presumption when applying a standard local error control is that the solution to the problem under consideration is regular enough such that no order reductions occur; in the latter case, error estimates cannot be expected to be asymptotically correct, but rather to display the same order as the basic integrator as mandated by the lack of smoothness.

We introduce pairs of related split-step formulae which provide estimates of the local error with moderate additional computational effort. Our methods are in the spirit of *embedded Runge–Kutta methods*, see for instance [6,14], where a pair of Runge–Kutta methods of different orders is constructed such that several of the internal stages coincide, whence the number of function evaluations is reduced accordingly. Comparison of the results computed by both formulae yields an estimate of the local truncation error and hence a basis for time stepsize selection. We propose a similar procedure in the context of splitting algorithms to obtain *embedded exponential operator splitting methods* for the approximate solution of (1),

$$u_{n+1} = \mathrm{e}^{a_1 h_n D_A} \mathrm{e}^{b_1 h_n D_B} \cdots \mathrm{e}^{a_s h_n D_A} \mathrm{e}^{b_s h_n D_B} u_n \approx u(t_{n+1}) = \mathrm{e}^{h_n D_{A+B}} u(t_n), \tag{2a}$$

$$\hat{u}_{n+1} = \mathrm{e}^{\hat{a}_1 h_n D_A} \mathrm{e}^{\hat{b}_1 h_n D_B} \cdots \mathrm{e}^{\hat{a}_{\hat{s}} h_n D_A} \mathrm{e}^{\hat{b}_{\hat{s}} h_n D_B} u_n \approx u(t_{n+1}) = \mathrm{e}^{h_n D_{A+B}} u(t_n), \tag{2b}$$

that is, pairs of splitting methods where some of the substeps coincide. We point out that it is essential with regard to stability issues that both splitting methods, the integrator and the local error estimator, are given in multiplicative form (and not in additive form). We further note that in the calculus of Lie derivatives the ordering of operators is formally reversed, see also (6), and that in an implementation of (2a) the nonlinear evolution operator $\mathrm{e}^{a_1 h_n D_A}$ will be applied first. The formulae (2) are constructed such that the orders are not equal; thus, the difference between the two results computed on a subinterval can be used as an estimate of the local error on that interval. As standard, the optimal time stepsize h_{opt} for a prescribed tolerance tol is then determined by a relation of the form (e.g. with $\alpha_{\max} = 1.5$, $\alpha_{\min} = 0.2$, $\alpha = 0.25$ for our computations)

$$h_{\mathrm{optimal}} = h \cdot \min\left(\alpha_{\max}, \max\left(\alpha_{\min}, \sqrt[p+1]{\alpha \cdot \frac{\mathrm{tol}}{\mathrm{err}_{\mathrm{local}}}}\right)\right), \tag{3}$$

involving the current time stepsize h, the local error estimate $\mathrm{err}_{\mathrm{local}}$, the order of consistency p of the integrator, and, possibly, additional constants chosen in accordance with the application under consideration, see [14,26]. The computational advantage of embedded exponential operator splitting methods is obvious. When the first substeps of the two formulae coincide, only the last steps have to be computed separately, while the coinciding steps are only computed once.

The construction of embedded exponential operator splitting methods requires the (numerical) solution of the (classical) order conditions [13,21,32]. With a sufficient number of degrees of freedom for both schemes and the additional algebraic constraints that some substeps for both methods should coincide, this yields a system of nonlinear algebraic equations which can be solved numerically. To demonstrate the feasibility of this approach, we construct a pair of orders 4(3) with real method coefficients based on an optimised fourth-order scheme by Blanes and Moan [4], where four of the seven substeps coincide; the arising system of polynomial equations is reduced using Gröbner bases to a system which can readily be solved numerically. The pair of orders 4(3) with real method coefficients is tailored for the time integration of nonlinear Schrödinger equations. As an illustration, we apply this embedded split-step pair to the two-dimensional cubic Schrödinger equation with focusing singularity, which features a blowup behaviour and implies the need for adaptive reduction of time stepsizes when approaching the blowup time. Furthermore, two related pairs of orders 4(3) with complex coefficients are constructed and applied to a nonlinear reaction–diffusion equation in three space dimensions where the dissipative nature of the problem calls for an adaptive increase of the time stepsizes.

In the present work, we restrict ourselves to the construction of pairs of orders $p(p-1)$, which we consider to be the most relevant case for practical purposes. In an adaptive time integration based on local error control, the higher-order time

integration method serves as a local error estimator in order to determine the optimal time stepsize; nevertheless, the time integration is usually performed by the higher-order method. Thus, in order to avoid underestimating the time stepsizes, we focus on pairs of orders $p(p-1)$. Furthermore, we do not elaborate on the numerical aspects of the highly nontrivial numerical solution of the associated algebraic equations and compute only pairs of moderate orders to illustrate the general principle. In particular the construction of methods with minimal error constants [4] leading to a high-dimensional optimisation problem is not in the scope of the present work.

The theoretical basis of the new algorithms in the context of (nonlinear) evolutionary equations, in particular in connection with (nonlinear) Schrödinger equations, is provided by the error analysis for higher-order exponential operator splitting methods given in [21,32]. The latter works extend the techniques exploited in the fundamental contributions [20,22], see also [10] for an alternative approach and [3,8,15] for split-step formulae involving complex coefficients. The theoretical investigations show that exponential operator splitting methods retain their orders of convergence when applied to evolution problems with sufficiently regular solutions; this is also in accordance with numerical observations. We point out that it is (rather) straightforward to carry out a theoretical (local) error analysis for the real order 4(3) split-step pair applied to the cubic Schrödinger equation utilising the techniques developed in [21,22]. More precisely, it (only) remains to specialise the local error expansion stated in [21, Theorem 2.1] for an abstract nonlinear evolution equation to the considered application, which, in essence, reduces to the calculation of higher-order iterated Lie-commutators of the involved operators, see also [21, Lemma 3.3]. Basic assumptions analogous to [21, Theorem 3.2] are certain regularity requirements on the analytical solution of the problem. Provided that these regularity requirements are satisfied, a favourable convergence behaviour of the order 4(3) split-step pair is obtained for the cubic Schrödinger equation, but otherwise an order reduction is encountered. It should be noted that similar concepts are applicable for problems of parabolic type. However, as we explain in Section 3.2, for this class of problems the effect of the imposed (for instance zero) boundary conditions, which are in many cases unnatural conditions on space derivatives of the analytical solution, may cause a significant order reduction. This negative influence on the good performance of splitting methods is in contrast to nonlinear Schrödinger equations such as Gross–Pitaevskii systems, where also derivatives of the (physically relevant) solution satisfy the imposed (for example asymptotic) boundary conditions.

The contents of this manuscript are as follows: Our main objective is the introduction of embedded exponential operator splitting methods for the reliable time integration of different types of nonlinear evolution equations, see Section 2. In particular, the scope of applications ranges from time-dependent nonlinear Schrödinger equations to nonlinear parabolic initial-boundary value problems. The general approach for the construction of new algorithms is illustrated on the basis of order 4(3) split-step pairs involving real or complex coefficients, respectively. Theoretical investigations and numerical examples for two model problems, the two-dimensional cubic Schrödinger equation and a three-dimensional nonlinear reaction–diffusion equation are given in Section 3. Furthermore, we include numerical illustrations for the time-dependent Gross–Pitaevskii equation to demonstrate good energy conservation by the use of an adaptive splitting method as well as a comparison of our real embedded 4(3) pair with the alternative use of an unrelated three-stage third-order scheme as local error estimator.

2. Embedded splitting methods for nonlinear evolutionary problems

2.1. Nonlinear evolutionary problems

In the following, we consider abstract initial value problems of the form

$$u'(t) = F\big(u(t)\big), \quad 0 \leqslant t \leqslant T, \quad u(0) \text{ given}, \tag{4a}$$

for Banach space-valued functions $u : [0,T] \to X$, where the structure of the (unbounded) nonlinear operator $F : D(F) \subset X \to X$ suggests a decomposition into two parts

$$F(v) = A(v) + B(v), \quad v \in D(A) \cap D(B), \tag{4b}$$

with (unbounded) nonlinear operators $A : D(A) \subset X \to X$ and $B : D(B) \subset X \to X$; throughout, we tacitly require that the domains are suitably chosen subspaces of the underlying Banach space $(X, \|\cdot\|_X)$ such that $\emptyset \neq D(A) \cap D(B) \subseteq D(F)$. Without loss of generality, we may restrict ourselves to autonomous differential equations, see for example [18].

Formally, the exact solution of the evolutionary problem (4) is given by

$$u(t) = \mathcal{E}_F\big(t, u(0)\big), \quad 0 \leqslant t \leqslant T, \tag{5a}$$

with the evolution operator $\mathcal{E}_F$ depending on time and the initial value. A most helpful tool in the statement and the theoretical analysis of high-order exponential operator splitting methods for nonlinear evolution equations is the formal calculus of Lie derivatives, where (5a) is recast as

$$u(t) = \mathrm{e}^{tD_F} u(0), \quad 0 \leqslant t \leqslant T, \tag{5b}$$

see [13,22] or [21] for a detailed exposition. More precisely, for an (unbounded) nonlinear operator $G : D(G) \subset X \to X$ (with suitable domain), the evolution operator e^{tD_F} and the Lie-derivative D_F are given by

$$e^{tD_F} G v = G\big(\mathcal{E}_F(t, v)\big), \quad 0 \leqslant t \leqslant T, \qquad D_F G v = G'(v) F(v); \tag{6}$$

if G is the identity operator, we write $e^{tD_F} v = \mathcal{E}_F(t, v)$ and $D_F v = F(v)$ for short.

2.2. Exponential operator splitting methods

The nonlinear evolutionary problem (4) is discretised in time by an exponential operator splitting method of (classical) order $p \geqslant 1$ involving $s \geqslant 1$ compositions. We employ the following general formulation of a splitting method that includes various example methods proposed in the literature.

Starting from an initial value $u_0 \approx u(0)$, numerical approximations to the exact solution values at time grid points $0 = t_0 < t_1 < \cdots < t_N \leqslant T$ with associated time stepsizes $h_n = t_{n+1} - t_n$, $0 \leqslant n \leqslant N-1$, are determined through a recurrence relation of the form

$$u_{n+1} = e^{a_1 h_n D_A} e^{b_1 h_n D_B} \cdots e^{a_s h_n D_A} e^{b_s h_n D_B} u_n \approx e^{t_{n+1} D_{A+B}} u(0) = u(t_{n+1}), \tag{7}$$

with real or complex method coefficients $(a_j, b_j)_{j=1}^{s}$, see also (6). We assume the procedure (7) to be well-defined on a suitably chosen function space.

To construct a splitting formula of a certain (classical) order $p \geqslant 1$, a system of algebraic equations for the method coefficients has to be solved. In the context of linear evolutionary Schrödinger equations, these order conditions are deduced in [32] and it is shown that they coincide with the well-known nonstiff order conditions, see also [21] for the nonlinear case.

As an illustration and in view of the example methods under consideration, the order conditions up to order $p = 3$ are given in formula (10) below.

Low-order example methods that can be cast into the scheme (7) are the first-order Lie–Trotter splitting method, where

$$\begin{aligned} &s = 1, \qquad a_1 = b_1 = 1, \quad \text{or} \\ &s = 2, \qquad a_1 = b_2 = 0, \qquad a_2 = b_1 = 1, \end{aligned} \tag{8}$$

respectively, and the widely used second-order symmetric Lie–Trotter or Strang splitting method, where

$$\begin{aligned} &s = 2, \qquad a_1 = a_2 = \frac{1}{2}, \qquad b_1 = 1, \qquad b_2 = 0, \quad \text{or} \\ &s = 2, \qquad a_1 = 0, \qquad a_2 = 1, \qquad b_1 = b_2 = \frac{1}{2}, \end{aligned} \tag{9}$$

respectively, see [30,34]. We note that the split-step formulae in (8) or (9), respectively, correspond to the same method with exchanged rôles of A and B.

Various higher-order example methods that were proposed in the literature are reviewed in [13,24]. For orders $p = 4, 6$, splitting methods of the ilk of Runge–Kutta–Nyström methods that are particularly favourable for Hamiltonian systems and Schrödinger equations are given in [4].

2.3. Embedded splitting methods

In order to estimate the local error of higher-order exponential operator splitting methods, we propose a computationally cheap method in the spirit of embedded Runge–Kutta methods [14]. We consider embedded split-step pairs $p(\hat{p})$ with coefficients

$$(a_j, b_j)_{j=1}^{s}, \qquad (\hat{a}_j, \hat{b}_j)_{j=1}^{\hat{s}}$$

where some of the compositions coincide. Thus, the difference between the two approximations

$$\begin{aligned} u_{n+1} &= e^{a_1 h_n D_A} e^{b_1 h_n D_B} \cdots e^{a_s h_n D_A} e^{b_s h_n D_B} u_n, \\ \hat{u}_{n+1} &= e^{\hat{a}_1 h_n D_A} e^{\hat{b}_1 h_n D_B} \cdots e^{\hat{a}_{\hat{s}} h_n D_A} e^{\hat{b}_{\hat{s}} h_n D_B} u_n, \end{aligned}$$

is used as a local error estimate. For a pair $p(\hat{p})$, we denote by p the order of the basic integrator and by $\hat{p}$ the order of the error estimator. Clearly, the rôles of p and $\hat{p}$ can be exchanged.

Table 1
Coefficients of a real embedded split-step pair of orders 4(3) based on a fourth-order scheme by Blanes and Moan [4].

j	a_j	j	b_j
1	0	1, 7	0.0829844064174052
2, 7	0.245298957184271	2, 6	0.3963098014983680
3, 6	0.604872665711080	3, 5	−0.0390563049223486
4, 5	$1/2-(a_2+a_3)$	4	$1-2(b_1+b_2+b_3)$
j	$\hat{a}_j$	j	$\hat{b}_j$
1	a_1	1	b_1
2	a_2	2	b_2
3	a_3	3	b_3
4	a_4	4	b_4
5	0.3752162693236828	5	0.4463374354420499
6	1.4878666594737946	6	−0.0060995324486253
7	−1.3630829287974774	7	0

Algorithm 1 *(Pair 2(1)).* A trivial embedded split-step pair is based on the second-order Strang splitting and the first-order Lie–Trotter splitting

$$a_1=0,\qquad a_2=1,\qquad b_1=b_2=\frac{1}{2},$$
$$\hat{a}_1=\hat{b}_2=0,\qquad \hat{a}_2=\hat{b}_1=1.$$

Algorithm 2 *(Pair 4(3)).* The coefficients of a split-step pair of orders 4(3) that is based on a fourth-order Runge–Kutta–Nyström type method given in [4] are specified in Table 1. We note that the basic 4th-order split-step method is optimised with regard to the effective error constant and shows favourable accuracy and efficiency when applied to the time-dependent Gross–Pitaevskii equation [7].

The construction of the embedded third-order split-step formula relies on the following approach: The order conditions to be satisfied for order $\hat{p}=3$ are

$$\sum_{j=1}^{\hat{s}}\hat{a}_j=1,\qquad \sum_{j=1}^{\hat{s}}\hat{b}_j=1,$$
$$\sum_{j=1}^{\hat{s}}\hat{b}_j\hat{c}_j=\frac{1}{2},$$
$$\sum_{j=1}^{\hat{s}}\hat{b}_j\hat{c}_j^2=\frac{1}{3},\qquad \frac{1}{2}\sum_{j=1}^{\hat{s}}\hat{b}_j^2\hat{c}_j+\sum_{j=1}^{\hat{s}}\sum_{k=1}^{j-1}\hat{b}_j\hat{b}_k\hat{c}_j=\frac{1}{3},\tag{10}$$

where $\hat{c}_j=\sum_{i=1}^{j}\hat{a}_i$ for $1\leqslant j\leqslant\hat{s}$. With the help of the computer algebra system Maple, we compute a reduced Gröbner basis of the above system of algebraic equations for $\hat{s}=7$ (requiring $\hat{b}_7=0$) with respect to the pure lexicographic ordering $(\hat{a}_5,\hat{a}_6,\hat{a}_7,\hat{b}_5,\hat{b}_6)$. In the resulting system of algebraic equations, we substitute the coefficients $\hat{a}_j=a_j$ as well as $\hat{b}_j=b_j$, $1\leqslant j\leqslant 4$. This yields a single quadratic equation for $\hat{b}_6$ and four linear equations for $\hat{a}_5$, $\hat{a}_6$, $\hat{a}_7$, $\hat{b}_5$, which can easily be solved numerically.

Algorithm 3 *(Complex pair 4(3)).* Two split-step pairs of orders 4(3) with four compositions involving complex method coefficients with non-negative real parts, suitable for the time integration of dissipative parabolic problems, are given in Table 2. Their construction, inspired by Yoshida's splitting formula of order four involving four compositions [13, p. 40, Formula (4.4)], is in the lines of Algorithm 2. In the present case, two alternative third-order formulae are found under the requirements $\hat{a}_1=a_1$, $\hat{b}_1=b_1$, and $\hat{b}_4=0$.

With the above example methods we intended to illustrate the general principle, but we do not claim to give formulae which are optimal for instance in terms of accuracy and efficiency. While for the real pair 4(3), eight of the 13 coefficients of the higher-order method also appear in the second formula, for the complex pair only two compositions are reused. A comparison of our real embedded 4(3) pair versus a pair comprising the fourth-order scheme by Blanes and Moan [4] and an unrelated three-stage third-order scheme is given in Section 3, which demonstrates that the embedded approach is favourable. The computation of higher-order splitting schemes is a highly challenging optimisation problem, which would exceed the scope of the present paper and is addressed by other authors, see for example the recent contribution [3].

Table 2
Coefficients of two complex embedded split-step pairs of orders 4(3). Integrator (top) and two alternative error estimators (middle, bottom).

j	a_j	j	b_j
1	0	1, 4	$0.1621982020100856 + 0.0672931362454034\mathrm{i}$
2, 4	$0.3243964040201712 + 0.1345862724908067\mathrm{i}$	2, 3	$0.3378017979899144 - 0.0672931362454034\mathrm{i}$
3	$0.3512071919596576 - 0.2691725449816134\mathrm{i}$		
j	$\hat{a}_j$	j	$\hat{b}_j$
1	a_1	1	b_1
2	$0.4157701540561051 + 0.2129482257474245\mathrm{i}$	2	$0.4052251807333103 + 0.1988642124619028\mathrm{i}$
3	$0.3855092282056243 - 0.1105557092016989\mathrm{i}$	3	$0.4325766172566041 - 0.2661573487073062\mathrm{i}$
4	$0.1987206177382706 - 0.1023925165457255\mathrm{i}$	4	0
j	$\hat{a}_j$	j	$\hat{b}_j$
1	a_1	1	b_1
2	$0.3846692310454507 - 0.0071358558333693\mathrm{i}$	2	$0.4325766172566041 - 0.2661573487073062\mathrm{i}$
3	$0.3855092282056243 - 0.1105557092016989\mathrm{i}$	3	$0.4052251807333103 + 0.1988642124619028\mathrm{i}$
4	$0.2298215407489250 + 0.1176915650350683\mathrm{i}$	4	0

3. Numerical examples

In the following, we give three numerical examples which serve to demonstrate that local error control based on our embedded splitting methods is feasible and generates a stepsize sequence which is commensurate with the solution behaviour. In all cases, the main computational task is the numerical integration of the linear part realised by pseudo-spectral methods, whereas the numerical approximation of the nonlinearity involves cheap pointwise multiplications.

3.1. Cubic Schrödinger equation

As a first illustration, we consider the cubic Schrödinger equation

$$\mathrm{i}\partial_t \psi(x,t) = -\frac{1}{2}\Delta\psi(x,t) + \vartheta\left|\psi(x,t)\right|^2\psi(x,t), \quad x \in \mathbb{R}^2,\ t \geqslant 0, \tag{11}$$

for the complex-valued function $\psi : \mathbb{R}^2 \times \mathbb{R}_{\geqslant 0} \to \mathbb{C} : (x,t) \mapsto \psi(x,t)$. For negative interaction parameters $\vartheta < 0$ a focusing singularity occurs which leads to a blowup behaviour and resulting need for adaptive reduction of time stepsizes close to the blowup time, where the solution becomes unbounded, see [31].

On the time interval where a regular solution to the cubic Schrödinger equation exists, a convergence result for higher-order exponential operator splitting methods was established in [21] for three spatial dimensions; the result includes error estimates in the Sobolev spaces $L^2(\mathbb{R}^3)$, $H^1(\mathbb{R}^3)$, and $H^2(\mathbb{R}^3)$. Since analogous Sobolev imbeddings $H^2(\mathbb{R}^2)$ in $L^\infty(\mathbb{R}^2)$ and $H^1(\mathbb{R}^2)$ in $L^4(\mathbb{R}^2)$, $L^6(\mathbb{R}^2)$ hold, see [1], the convergence analysis also applies to our test problem. In particular, Theorem 1 shows that high-order splitting methods retain their (nonstiff) orders of convergence, provided that the solution to (11) is sufficiently regular.

Theorem 1. *Suppose that the cubic nonlinear Schrödinger equation (11) possesses a uniquely determined and sufficiently regular solution $\psi : [0,T] \to \mathbb{C}$. Then, for any exponential operator splitting method (7) of order $p \geqslant 2$, the following error bounds hold.*

(i) *If $\|\psi(t)\|_{H^{2p-2}} \leqslant M_{2p-2}$ for $0 \leqslant t \leqslant T$, the estimate*

$$\left\|u_n - \psi(t_n)\right\|_{H^2} \leqslant Ch^{p-2}, \quad 0 \leqslant n \leqslant N, \quad t_N \leqslant T,$$

is valid with constant C depending on M_{2p-2}.

(ii) *If $\|\psi(t)\|_{H^{2p-1}} \leqslant M_{2p-1}$ for $0 \leqslant t \leqslant T$, the estimate*

$$\left\|u_n - \psi(t_n)\right\|_{H^1} \leqslant Ch^{p-1}, \quad 0 \leqslant n \leqslant N, \quad t_N \leqslant T,$$

is valid with constant C depending on M_{2p-1}.

(iii) *If $\|\psi(t)\|_{H^{2p}} \leqslant M_{2p}$ for $0 \leqslant t \leqslant T$, the estimate*

$$\left\|u_n - \psi(t_n)\right\|_{L^2} \leqslant Ch^{p}, \qquad 0 \leqslant n \leqslant N, \quad t_N \leqslant T,$$

is valid with constant C depending on M_{2p}.

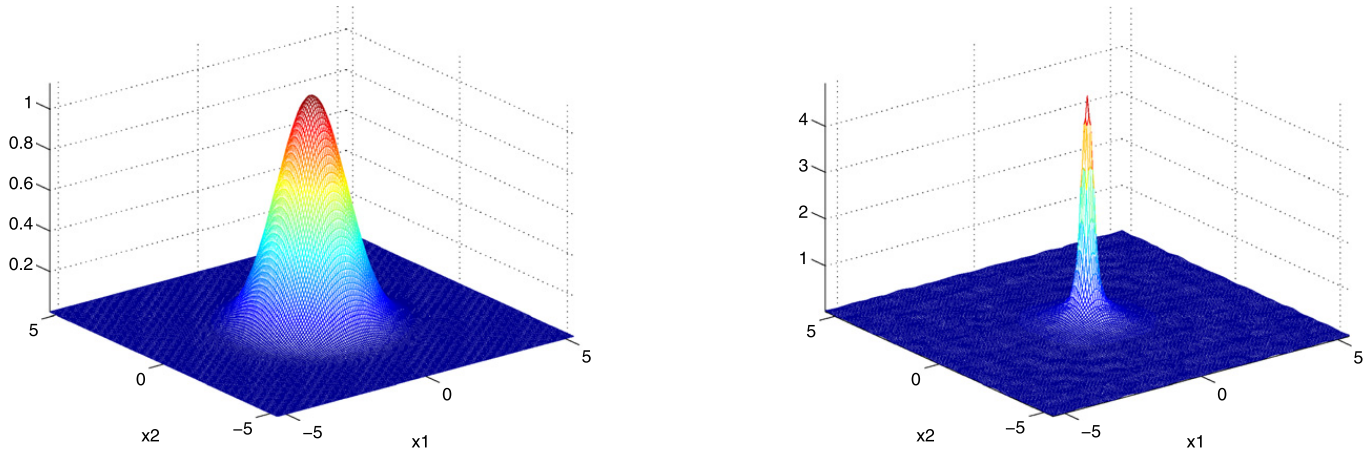

Fig. 1. Solution profile $|\psi(x,t)|$ of the cubic Schrödinger equation (11) at initial time $t=0$ and final time $t=10$.

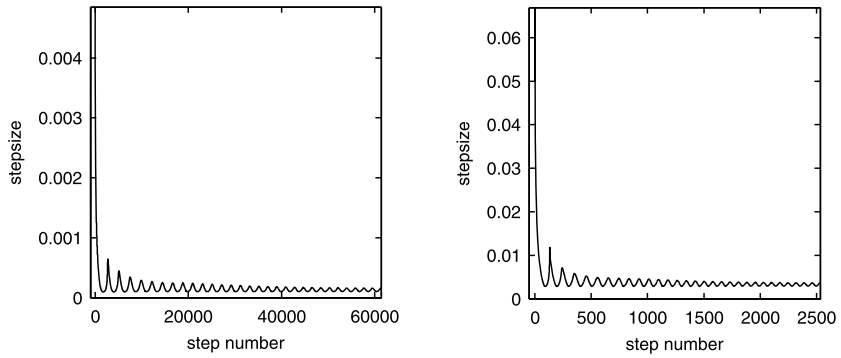

Fig. 2. Time integration of the cubic Schrödinger equation (11). Adaptive reduction of the time stepsizes for the split-step pair 2(1) (left) and the split-step pair 4(3) (right), respectively.

Table 3
Empirical convergence orders of the fourth-order (left) and third-order (right) split-step methods given in Table 1 applied to the cubic Schrödinger equation (11).

Δt	Global error	Order	Δt	Global error	Order
2^{-5}	$1.15\cdot 10^{-2}$	4.98	2^{-5}	$8.02\cdot 10^{-2}$	2.57
2^{-6}	$3.64\cdot 10^{-4}$	5.49	2^{-6}	$1.35\cdot 10^{-2}$	3.11
2^{-7}	$8.11\cdot 10^{-6}$	5.07	2^{-7}	$1.57\cdot 10^{-3}$	3.20
2^{-8}	$2.41\cdot 10^{-7}$	4.47	2^{-8}	$1.71\cdot 10^{-4}$	2.99
2^{-9}	$1.09\cdot 10^{-8}$	4.13	2^{-9}	$2.16\cdot 10^{-5}$	2.96
2^{-10}	$6.20\cdot 10^{-10}$	3.89	2^{-10}	$2.78\cdot 10^{-6}$	3.13

For our numerical test, we use a spatial semi-discretisation based on the Fourier spectral method with 128×128 basis functions on $[-16,16]\times[-16,16]$; for the time integration on $[0,10]$ the embedded split-step pair of orders 4(3) given in Table 1 is applied, see also (3) for the selection of the optimal time stepsize. We note that the underlying fourth-order method [4] is symmetric and may therefore be more suitable as the basic geometric integrator for Schrödinger equations.

In Fig. 1, the chosen initial value $\psi(x,0)=2\pi^{-\frac{1}{2}}\mathrm{e}^{-\frac{1}{2}|x|^2}$ as well as the modulus of the numerical solution of (11) with $\vartheta=-2$ at final time $t=10$ are given; note the typical blowup behaviour resulting in an increasing L^∞-norm of the solution, whereas the L^2-norm remains conserved. To better resolve the singularity at the origin, spatial adaptivity would be mandatory; on our fixed space grid the size of the solution which can be observed remains moderate.

The empirical convergence orders of the fourth-order and third-order split-step methods at time $t=1$ are displayed in Table 3; a reference solution is computed with constant time stepsize $\Delta t=2^{-11}$.

For an absolute tolerance $\mathrm{tol}=10^{-4}$, the adaptive selection of time stepsizes is shown in Fig. 2; for comparison, we also include the result for the split-step pair of orders 2(1), see Algorithm 1. We observe that the time stepsizes are commensurate with the evolution of the solution profile. As expected, the fourth-order splitting method is superior to the low-order integrator when strict tolerances are imposed.

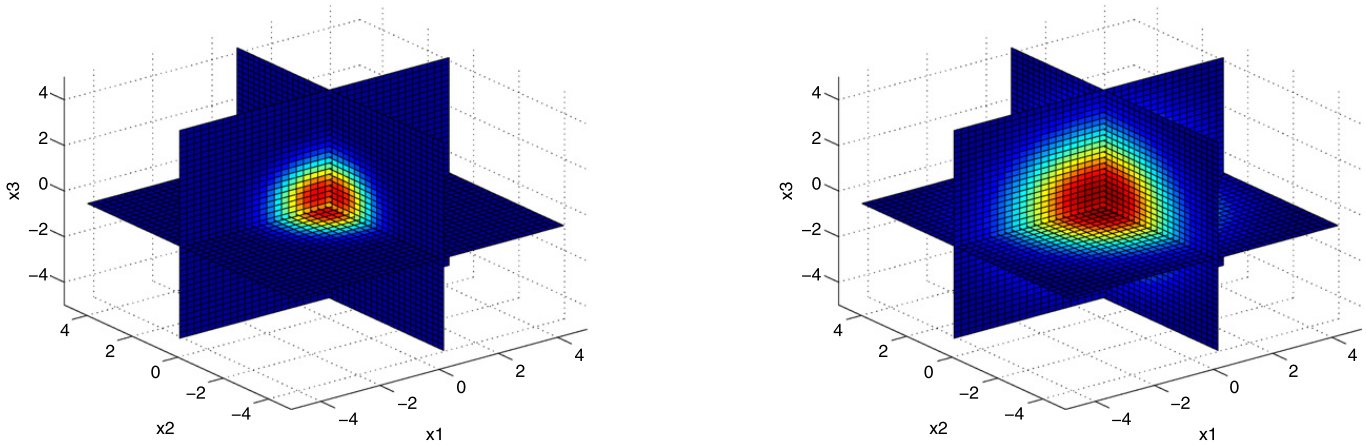

Fig. 3. Solution $u(x,t)$ of the parabolic problem (12) at initial time $t=0$ and final time $t=1$.

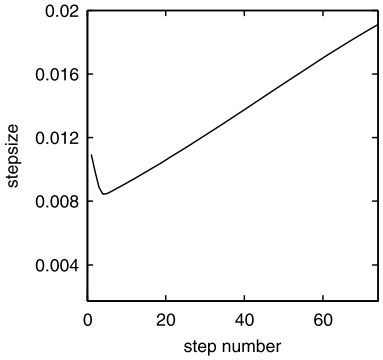

Fig. 4. Time integration of the parabolic problem (12). Adaptive growth of the time stepsizes for the complex split-step pair 4(3).

3.2. Parabolic problem

As our second illustration, we consider the reaction–diffusion equation

$$\partial_t u(x,t) = \frac{1}{2}\Delta u(x,t) + u(x,t)\big(1-u(x,t)\big), \quad x\in\Omega, \quad t\geqslant 0, \tag{12}$$

for the real-valued function $u:\Omega\times\mathbb{R}_{\geqslant 0}\to\mathbb{R}:(x,t)\mapsto u(x,t)$, subject to homogeneous Dirichlet boundary conditions on a bounded domain $\Omega\subset\mathbb{R}^3$.

In order to establish a convergence result for higher-order splitting methods applied to evolutionary problems of parabolic type, in principle, the approach is the same as for the cubic Schrödinger equation; but, as mentioned below, the imposed boundary conditions will in general lead to order reduction phenomena. However, in the present test example, we may neglect this effect; due to the Hölder and Sobolev inequalities [16,5], it follows

$$\big\|u^2\big\|_{L^2} \leqslant \|u\|_{L^4}^2 \leqslant C\|u\|_{H^1}^2,$$

and thus we can establish a convergence bound under the same regularity requirements on the solution as in Theorem 1. Again, this shows that the (nonstiff) convergence order of splitting methods is retained.

In the numerical solution process, the dissipativity of the problem allows to increase the time stepsizes adaptively, see Fig. 4.

We employ a spatial semi-discretisation based on the sine spectral method with $64\times 64\times 64$ basis functions on $[-8,8]\times[-8,8]\times[-8,8]$; for the time integration on $[0,1]$ the embedded complex split-step pair of orders 4(3) given in Table 2 (top, middle) is applied.

In Fig. 3, the chosen initial value $u(x,0)=\pi^{-\frac{3}{4}}\mathrm{e}^{-\frac{1}{2}|x|^2}$ as well as the numerical solution of (12) at time $t=1$ are given; the figure displays the value of $u(x,t)$ represented by the color code along slices defined by the three planes $x_1=\frac{1}{2}$, $x_2=\frac{1}{2}$, and $x_3=-\frac{1}{2}$.

The empirical convergence orders of the fourth-order and third-order complex split-step methods at time $t=1$ are illustrated in Table 4; a reference solution is computed with constant time stepsize $\Delta t=2^{-7}$. Note that the initial value and its higher derivatives satisfy the homogeneous boundary conditions on the considered spatial domain (to sufficient accuracy); however, for a smaller domain this might be violated whence an order reduction would ensue.

For an absolute tolerance $\mathrm{tol}=10^{-10}$, the adaptive growth of time stepsizes is shown in Fig. 4.

Table 4
Empirical convergence orders of the fourth-order (left) and third-order (right) complex split-step methods given in Table 2 (top, middle) applied to the parabolic problem (12).

Δt	Global error	Order	Δt	Global error	Order
2^{-1}	$1.80 \cdot 10^{-3}$	3.07	2^{-1}	$3.06 \cdot 10^{-3}$	2.43
2^{-2}	$2.16 \cdot 10^{-4}$	3.54	2^{-2}	$5.66 \cdot 10^{-4}$	2.73
2^{-3}	$1.86 \cdot 10^{-5}$	3.83	2^{-3}	$8.53 \cdot 10^{-5}$	2.91
2^{-4}	$1.31 \cdot 10^{-6}$	3.95	2^{-4}	$1.14 \cdot 10^{-5}$	2.98
2^{-5}	$8.49 \cdot 10^{-8}$	3.99	2^{-5}	$1.45 \cdot 10^{-6}$	3.01
2^{-6}	$5.34 \cdot 10^{-9}$	4.08	2^{-6}	$1.79 \cdot 10^{-7}$	3.17

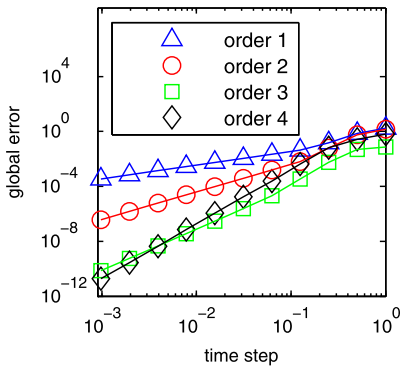

Fig. 5. Global errors at $t = 1$ of the Lie splitting (order 1), the Strang splitting (order 2), and the real embedded splitting pair (orders 3 and 4) applied to the one-dimensional Gross–Pitaevskii equation with $\varepsilon = 1$.

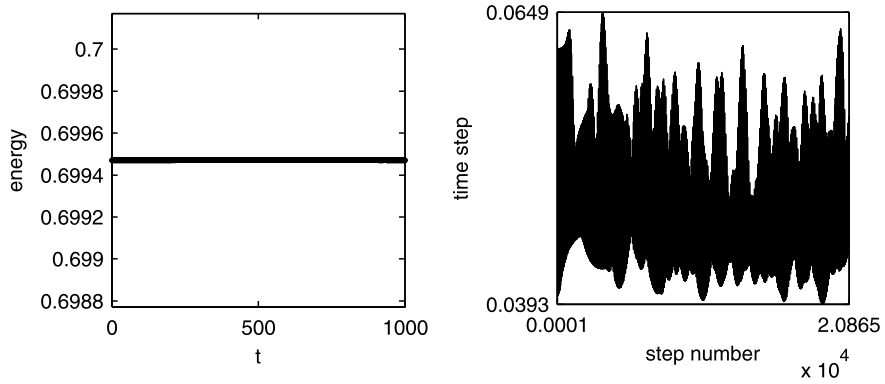

Fig. 6. Time integration of the Gross–Pitaevskii equation (13) with $\varepsilon = 1$ by the real split-step pair 4(3). Energy versus time (left) and generated time steps (right).

3.3. Gross–Pitaevskii equation

Finally, we consider the one-dimensional Gross–Pitaevskii equation

$$\begin{cases} \mathrm{i}\partial_t \psi(x,t) = -\dfrac{1}{2}\partial_{xx}\psi(x,t) + V(x)\psi(x,t) + \vartheta\left|\psi(x,t)\right|^2\psi(x,t), \\ \psi(x,0) \text{ given}, \quad x \in \mathbb{R}, \quad t \geqslant 0, \end{cases} \tag{13}$$

governed by a harmonic external potential $V(x) = \frac{1}{2}x^2$. A convergence result analogous to Theorem 1 is given in [12,33].

As a first illustration, the global error of the first-order Lie–Trotter splitting method, the second-order Strang splitting method, and the real splitting schemes of orders three and four forming the embedded pair are displayed in Fig. 5. For the space discretisation, we apply the Fourier spectral method with 512 basis functions on the space interval $[-8, 8]$. Note that the slopes of the lines reflect the true orders of convergence and that the third-order scheme is favourable in accuracy compared to the optimised fourth-order scheme proposed by Blanes and Moan.

The time integration, starting from an initial (normalised) Gaussian, is performed by the real embedded split-step pair of orders 4(3) with tolerance 10^{-6}. In Fig. 6, we display the results for the energy showing good conservation properties and the underlying automatically generated time stepsizes for $t \in [0, 1000]$.

Table 5
Time integration of the Gross–Pitaevskii equation (13) with $\varepsilon = 1$. Global errors at time $T = 1$ of the third-order method associated with the real split-step pair 4(3) given in Table 1 (left) and the three-stage third-order scheme (14) (right).

Δt	Global error	Δt	Global error
1	$1.06 \cdot 10^{-2}$	1	$2.82 \cdot 10^{-2}$
2^{-1}	$1.24 \cdot 10^{-3}$	2^{-1}	$3.00 \cdot 10^{-3}$
2^{-2}	$1.75 \cdot 10^{-4}$	2^{-2}	$3.32 \cdot 10^{-4}$
2^{-3}	$2.19 \cdot 10^{-5}$	2^{-3}	$3.57 \cdot 10^{-5}$
2^{-4}	$2.77 \cdot 10^{-6}$	2^{-4}	$4.36 \cdot 10^{-6}$
2^{-5}	$3.48 \cdot 10^{-7}$	2^{-5}	$5.41 \cdot 10^{-7}$
2^{-6}	$4.36 \cdot 10^{-8}$	2^{-6}	$6.74 \cdot 10^{-8}$
2^{-7}	$5.45 \cdot 10^{-9}$	2^{-7}	$8.42 \cdot 10^{-9}$
2^{-8}	$6.82 \cdot 10^{-10}$	2^{-8}	$1.05 \cdot 10^{-9}$
2^{-9}	$8.53 \cdot 10^{-11}$	2^{-9}	$1.31 \cdot 10^{-10}$
2^{-10}	$1.07 \cdot 10^{-11}$	2^{-10}	$1.64 \cdot 10^{-11}$

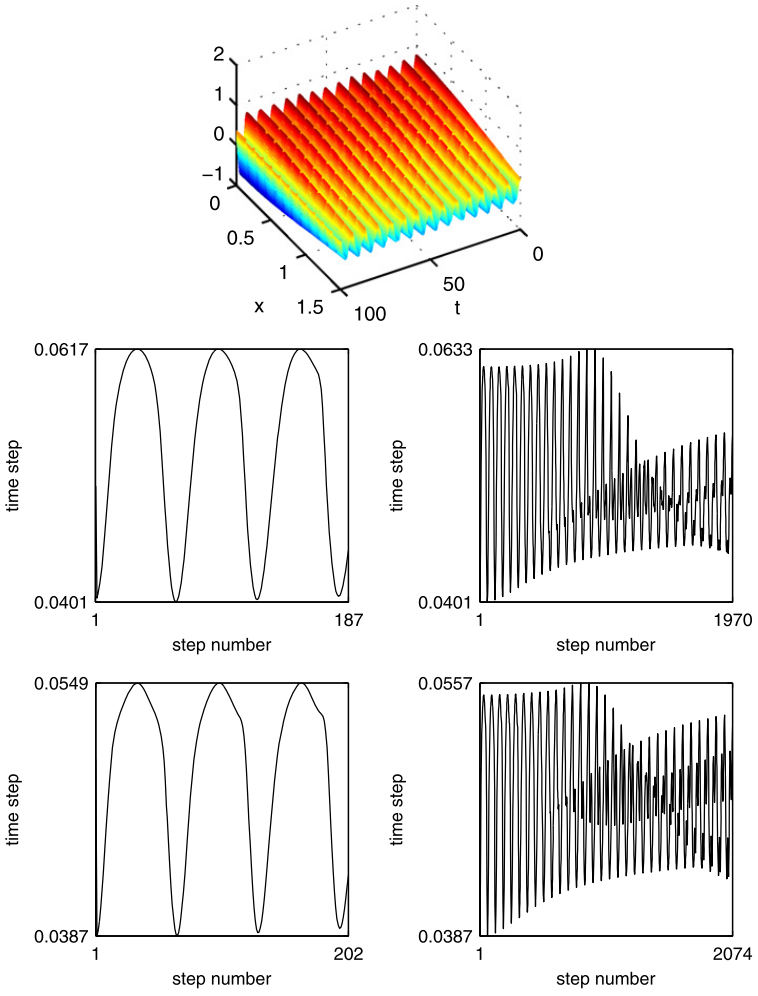

Fig. 7. Time integration of the Gross–Pitaevskii equation (13) with $\varepsilon = 1$. First row: Solution profile $\Re\psi$ for the section $(x,t) \in [0, 1.5] \times [0, 100]$. Second row: Time stepsizes for $t \in [0, 10]$ (left) and $t \in [0, 100]$ generated by the real split-step pair 4(3). Third row: Time stepsizes for $t \in [0, 10]$ (left) and $t \in [0, 100]$ generated by the split-step pair 4(3) with unrelated three-stage third-order scheme.

A naive local error control could be based on a pair comprising again the optimised fourth-order scheme by Blanes and Moan [4] and an unrelated three-stage third-order scheme with real coefficients

$$a_1 = 1, \qquad a_2 = -\frac{2}{3}, \qquad a_3 = \frac{2}{3}, \quad b_1 = -\frac{1}{24}, \qquad b_2 = \frac{3}{4}, \qquad b_3 = \frac{7}{24}. \tag{14}$$

However, as the results displayed in Table 5 and Fig. 7 confirm, such a choice does not compare favourably to the constructed embedded pair: The latter scheme has a larger effective error constant and thus induces smaller time steps at the same cost for each step.

4. Conclusions

We have put forward embedded exponential operator splitting time integration methods for nonlinear evolution equations. The new algorithms are constructed in a similar manner to embedded Runge–Kutta pairs such as to yield a computationally cheap estimate of the local error by reusing several of the substeps in two methods of different orders. To exemplify the principle, we have constructed pairs of orders 4(3) with real coefficients which are suitable for the solution of Schrödinger equations and pairs of the same orders with complex coefficients, appropriate for parabolic problems. Furthermore, we have demonstrated that adaptive stepsize selection can successfully be based on these methods. To this end, numerical illustrations for the cubic nonlinear Schrödinger equation in two space dimensions, a nonlinear parabolic problem in three space dimensions, and the one-dimensional Gross–Pitaevskii equation have been included.

Interesting aspects for future investigations are the construction of favourable embedded split-step pairs of higher-order and thorough numerical comparisons with alternative local error estimators based for instance on defect-correction [2] or extrapolation techniques.

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