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An Embedded Split-Step method for solving the nonlinear Schrödinger equation in optics

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Abstract

In optics the nonlinear Schrödinger equation (NLSE) which modelize wave propagation in an optical fiber is the most widely solved by the Symmetric Split-Step method. The practical efficiency of the Symmetric Split-Step method is highly dependent on the computational grid points distribution along the fiber, therefore an efficient adaptive step-size control strategy is mandatory. The most common approach for step-size control is the “step-doubling” approach. It provides an estimation of the local error at each computational grid point in order to set the next grid point in the best way to match a user predefined tolerance. The step-doubling approach increases of around 50 % the computational cost of the Symmetric Split-Step method. Alternatively there exists in optics literature other approaches based on the observation along the propagation length of the behavior of a given optical quantity. The step-size at each computational step is set so as to guarantee that the known properties of the quantity are preserved. These approaches derived under specific physical assumptions are low cost but suffer from a lack of generality. In this paper we present a new method for estimating the local error in the Symmetric Split-Step method when solving the NLSE. It conciliates the advantages of the step-doubling approach in term of generality and rigor but without the drawback of requiring a significant extra computational cost. The method is related to Embedded Split-Step methods for nonlinear evolution problems.

Keywords: Symmetric Split-Step method, adaptive step-size control, Nonlinear Schrödinger Equation

2000 MSC: 35Q55, 35Q60, 65M99

1. Introduction

The nonlinear Schrodinger equation (NLSE) describes a wide class of physical phenomena among which propagation of light in an optical fiber. We are concerned by the following form of the NLSE (see [1, 2])

$$\frac{\partial}{\partial z} A(z, t) = -\frac{\alpha}{2} A(z, t) + \left(\sum_{n=2}^N i^{n+1} \frac{\beta_n}{n!} \frac{\partial^n}{\partial t^n} A(z, t) \right) + i\gamma A(z, t) |A(z, t)|^2 \quad (1)$$

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where the complex valued function A represents the slowly varying pulse envelope of a quasi-monochromatic optical wave at frequency ω_0 in a frame of reference moving with the pulse at the group velocity $v_g = c/n_g$ where n_g denotes the group index of the fiber, z represents the position along the fiber and t the time in the local frame. In the situation considered here, the optical wave is assumed to be an electric field \mathbf{E} at frequency ω_0 which is linearly polarized along the vector \mathbf{e}_x transverse to the propagation's direction \mathbf{e}_z defined by the fiber axis and expressed as a function of position $\mathbf{r} = (x, y, z)$ and time τ in the form

$$\mathbf{E}(\mathbf{r}, \tau) = A(z, t) F(x, y) e^{-i(\omega_0 \tau - kz)} \mathbf{e}_x \quad (2)$$

where $F(x, y)$ is the electric wave transverse representation also called the ‘‘modal distribution’’ and k is the wavenumber. The relation between the ‘‘local time’’ t in the local frame and the absolute time τ is $t = \tau - z/v_g$.

Equation (1) describes wave propagation in a single mode fiber taking into account phenomena such as the optical Kerr effect through the nonlinear coefficient γ and linear dispersion through the dispersion coefficients β_n , $n = 2, \dots, N$ with $N \in \mathbb{N}$, $N \geq 2$. The coefficient α accounts for attenuation or gain during propagation in the fiber. The partial differential equation (PDE) (1) is to be solved for all z in a given interval $[0, L]$ where L denotes the length of the fiber and for all ‘‘local time’’ $t \in \mathbb{R}$. It is considered together with the following boundary condition at $z = 0$: $\forall t \in \mathbb{R}$, $A(0, t) = a_0(t)$, where a_0 is a given complex valued function.

The most widely used numerical method for solving the NLSE in optics is the Symmetric Split-Step method, see e.g. [3–7], due to its particular simplicity and efficiency. The idea behind the Symmetric Split-Step method applied to the NLSE (1) is to decompose over each subinterval of a given subdivision of the fiber length the PDE problem into a sequence of 3 simpler problems connected to each others. The first one corresponding to a purely linear PDE over the first half of the subinterval, the second one over the whole subinterval corresponding to a nonlinear ordinary differential equation (ODE) with the time variable as a parameter and the third one a purely linear PDE over the second half of the subinterval. The Symmetric Split-Step method applied to the NLSE (1) is detailed in section 2. The interest of this numerical approach for computing an approximation of the solution to the NLSE (1) is that each of the 3 nested problems can be solved more easily than equation (1) and when the step-size tends toward 0 the approximate solution is likely to converge to the solution of the NLSE (1).

It can be convenient for numerical simulation purposes to consider a normalized version of the NLSE (1). This can be achieved by introducing the normalized variables $t' = t/T_0$ and $z' = z/L_D$ where T_0 is the half-width of the source slowly varying pulse envelope a_0 and $L_D = T_0^2/|\beta_2|$ is known as the dispersion length [1]. When normalizing the slowly varying pulse envelope to the square root of its peak power P_0 , the new unknown $A'(z', t')$ is found to satisfy the following equation

$$\frac{\partial}{\partial z'} A'(z', t') = -\frac{\alpha'}{2} A'(z', t') + \left(\sum_{n=2}^N i^{n+1} \frac{\beta'_n}{n!} \frac{\partial^n}{\partial t'^n} A'(z', t') \right) + i\gamma' A'(z', t') |A'(z', t')|^2 \quad (3)$$

for $t' \in \mathbb{R}$ and $z' \in [0, L/L_D]$ where $\alpha' = L_D \alpha$, $\gamma' = L_D P_0 \gamma$ and $\beta'_n = (L_D/T_0^n) \beta_n$.

Let us now introduce a comprehensive mathematical framework for the study of our embedded Split-Step method applied to the NLSE. We denote by $\mathbb{L}^p(I, \mathbb{C})$, $p \in [1, +\infty[$ the set of complex-valued functions over the real interval I whose p -th powers are integrable and by $\mathbb{H}^m(I, \mathbb{C})$ for $m \in \mathbb{N}^*$ the Sobolev space of functions in $\mathbb{L}^2(I, \mathbb{C})$ with derivatives up to order m in

$\mathbb{L}^2(I, \mathbb{C})$, see e.g. [8]. For convenience, we will also use the notation $\mathbb{H}^0(I, \mathbb{C})$ for $\mathbb{L}^2(I, \mathbb{C})$ and $\mathbb{L}^\infty(I, \mathbb{C})$ for the space of essentially bounded functions. The Sobolev spaces $\mathbb{H}^m(I, \mathbb{C})$, $m \in \mathbb{N}$, are equipped with the usual norms denoted $\|\cdot\|_m$. For a function $A : (z, t) \in \mathbb{R}^2 \mapsto A(z, t) \in \mathbb{C}$, we denote by $A(z)$ the first partial function of A in z , i.e. $A(z) : t \in \mathbb{R} \mapsto A(z, t) \in \mathbb{C}$. The NLSE (1) can be reformulated as

$$\frac{\partial}{\partial z} A(z) = \mathcal{D}A(z) + \mathcal{N}(A(z)) \quad \forall z \in [0, L] \quad (4)$$

where the linear operator \mathcal{D} given by

$$\mathcal{D} : A(z) \mapsto \sum_{n=2}^N \beta_n \frac{i^{n-1}}{n!} \partial_t^n A(z) \quad (5)$$

is an unbounded linear operator on $\mathbb{L}^2(\mathbb{R}, \mathbb{C})$ with domain $\mathbb{H}^N(\mathbb{R}, \mathbb{C})$ and the non-linear operator \mathcal{N} given by

$$\mathcal{N} : A(z) \in \mathbb{L}^6(\mathbb{R}, \mathbb{C}) \mapsto -\frac{1}{2}\alpha A(z) + i\gamma A(z)|A(z)|^2 \in \mathbb{L}^2(\mathbb{R}, \mathbb{C}) \quad (6)$$

is locally Lipschitz continuous on every Sobolev space $\mathbb{H}^m(\mathbb{R}, \mathbb{C})$ for all $m \in \mathbb{N}^*$ with additionally $\mathcal{N} \in \mathbb{C}^\infty(\mathbb{H}^m(\mathbb{R}, \mathbb{C}), \mathbb{H}^m(\mathbb{R}, \mathbb{C}))$, see [9]. It can be seen that another splitting for the NLSE (1) is possible: the term $-\frac{1}{2}\alpha A$ can be added to the linear operator \mathcal{D} instead of the nonlinear operator \mathcal{N} .

For all $(k, m) \in \mathbb{N}^2$ and $I \subset \mathbb{R}$, we denote by $\mathbb{C}^k(I; \mathbb{H}^m(\mathbb{R}, \mathbb{C}))$ the space of functions $u : z \in I \mapsto u(z) \in \mathbb{H}^m(\mathbb{R}, \mathbb{C})$ with continuous derivatives up to order k (or just continuous when $k = 0$). When $N = 2$, a comprehensive mathematical framework for the NLSE (1) exists in the literature [10] and it is known that for $a_0 \in \mathbb{H}^2(\mathbb{R}, \mathbb{C})$ there exists a unique A belonging to $\mathbb{C}^0(\mathbb{R}; \mathbb{H}^2(\mathbb{R}, \mathbb{C})) \cap \mathbb{C}^1(\mathbb{R}; \mathbb{L}^2(\mathbb{R}, \mathbb{C}))$ solution of equation (1) satisfying $A(0) = a_0$. This result has been extended to an arbitrary value of N in [11]. Namely, denoting for any $m \in \mathbb{N}$ by $E_{m,N}(I)$ the space $\bigcap_{k=0}^{\lfloor m/N \rfloor} \mathbb{C}^k(I, \mathbb{H}^{m-Nk}(\mathbb{R}, \mathbb{C}))$, where $\lfloor s \rfloor$ denotes the integer part of $s \in \mathbb{R}^+$, the following result holds [11].

Theorem 1.1. *For all $a_0 \in \mathbb{H}^m(\mathbb{R}, \mathbb{C})$, with $m \in \mathbb{N}^*$, there exists a unique maximal solution $A \in E_{m,N}([0, Z])$, with $Z \in]0, +\infty]$, to the NLSE (1) with the initial condition $A(0) = a_0$ at $z = 0$. This solution satisfies*

$$\|A(z)\|_0 = e^{-\frac{\alpha}{2}z} \|a_0\|_0 \quad \text{for all } z \in [0, Z]. \quad (7)$$

Moreover, if N is even and $m \geq N/2$ then the solution is global, i.e. $Z = +\infty$.

As a corollary of theorem 1.1 we have that when N is an even integer and $a_0 \in \mathbb{H}^N(\mathbb{R}, \mathbb{C})$ the NLSE (1) with the initial condition $A(0) = a_0$ at $z = 0$ has a unique solution in the space $\mathbb{C}^0([0, L]; \mathbb{H}^N(\mathbb{R}, \mathbb{C})) \cap \mathbb{C}^1([0, L]; \mathbb{L}^2(\mathbb{R}, \mathbb{C}))$.

Of course, the practical efficiency of a numerical method such as the Symmetric Split-Step method applied to the NLSE (1) highly depends on the distribution of the computational grid points along the fiber and the use of an adaptive step-size control strategy is mandatory. The idea behind an adaptive step-size strategy is to introduce the grid points during the progress of the computation taking into account the information available at the current computation stage in order to determine the best suited step size (and therefore the next grid point) so as to maintain a given predefined accuracy of the approximation. Since it is not possible in practice to know the final global error, the step-size is determined so that a "local error" is lower than a prescribed

tolerance. In the literature dedicated to optics, a variety of adaptive step-size strategies have been proposed to be used in conjunction with Split-Step methods. We can distinguish 2 types of approaches. The one based on physical concepts (or physical intuition) where at each grid point the step-size is chosen so as a "local error" related quantity estimated from a physical quantity matches the prescribed tolerance value. For instance, in the so-called "nonlinear phase rotation method" [4] the step-size is chosen so that the phase change due to nonlinearity does not exceed a certain limit. In the "walk-off" method, the step-size is chosen to be inversely proportional to the product of the absolute value of the dispersion and the spectral bandwidth of the signal and the method applies to low power, multichannel systems [4]. In [12, 13] a method termed the "uncertainty principle method" is proposed where the determination of the step-size is done from the values of a parameter derived from an inequality which in quantum mechanics gives rise to the uncertainty principle between two non commuting operators. In [14] it is made use of the conservation of the "optical photon number" to estimate a local error related quantity and to define an adaptive step-size control strategy termed the Conservation Quantity Error method. This method applies to low loss fibers.

Another approach for defining adaptive step-size strategies consists in using purely numerical concepts. The "local error" is then defined as the error made using the numerical scheme when computing an approximation of the solution at the current grid point under the assumption that the value at the previous grid point was exact. In [4] the authors propose to use the "step-doubling" concept (see e.g. [15]) to estimate the local error when solving the NLSE by the Symmetric Split-Step method. This approach is closely related to the Step-Doubling method for local error estimation when numerically solving ordinary differential equations [16]. The main advantage of such an approach is that since no assumption on the physical parameters involved in the equation is made, the step-size strategy applies to an arbitrary set of parameters in the NLSE. However a drawback of the Step-Doubling method is a computational over-cost of approximately 50 % (when compared to the same Split-Step method with the "optimal" grid points distribution given in advance).

In this paper we propose an other way of estimating the local error in the Symmetric Split-Step method. The over-cost of the propound method is low. As for the Step-Doubling method, 2 approximate solutions of the NLSE corresponding to a "fine" solution and to a "coarse" solution are combined in a specific way to deliver a local error estimate. However, whereas in the Step-Doubling method the 2 approximate solutions are obtained by the use of the Symmetric Split-Step method on 2 mesh grids, the finest one having twice the number of grid points of the coarse one, our method uses the same mesh grid but 2 Split-Step schemes of different order: we use the Symmetric Split-Step scheme which is known to have second order of accuracy with a dedicated first order of accuracy Split-Step scheme. In order to reduce the over-cost for estimating the local error, the idea is to re-use some of the computations required by the Symmetric Split-Step scheme when computing the coarse solution by the first order Split-Step scheme. The first order Split-Step scheme is therefore non-conventional and has been designed to meet this goal. Although used in a different context, this approach is very similar to the one of embedded Runge-Kutta method for solving ordinary differential equations [17, 18]. It is also related to the embedded Split-Step formulae for the time integration of nonlinear evolution equation presented in [19].

The paper is organized as follows. In Section 2 we recall some of the features of the Symmetric Split-Step method useful for understanding the way the local error is estimated in our embedded Split-Step method. In Section 3 we present a first order Split-Step scheme embedded in the Symmetric Split-Step scheme designed to deliver a local error estimate at a very cheap cost. In Section 4 the algorithm of our Embedded Split-Step method and the underlying step-

size control strategy are detailed. Finally, in Section 5 we achieve a numerical comparison of our method with the Step-Doubling method on benchmark problems in optics.

2. Overview of the Symmetric Split-Step method

2.1. The Symmetric Split-Step scheme applied to the NLSE

In the Symmetric Split-Step scheme applied to the NLSE (1), the interval $[0, L]$ is divided into K subintervals where the spatial grid points are denoted z_k , $k \in \{0, \dots, K\}$, where $0 = z_0 < z_1 < \dots < z_{K-1} < z_K = L$. We also denote by $h_k = z_{k+1} - z_k$ the step-size between grid points z_k and z_{k+1} and we set $z_{k+\frac{1}{2}} = z_k + \frac{h_k}{2}$. The Symmetric Split-Step method applied to the NLSE (1) consists of solving over each subinterval $[z_k, z_{k+1}]$ for $k \in \{0, \dots, K-1\}$, the following 3 nested problems with time variable t as a parameter and the operators \mathcal{D} and \mathcal{N} defined as in (5) and (6):

$$\begin{cases} \frac{\partial}{\partial z} A_k^+(z) = \mathcal{D} A_k^+(z) & \forall z \in [z_k, z_{k+\frac{1}{2}}] \\ A_k^+(z_k) = A_{k-1}^{[2]}(z_k) \end{cases} \quad (8)$$

where $A_{k-1}^{[2]}(z_k)$ represents the approximate solution at grid point z_k computed by the Symmetric Split-Step method at step $k-1$;

$$\begin{cases} \frac{\partial}{\partial z} B_k(z) = \mathcal{N}(B_k(z)) & \forall z \in [z_k, z_{k+1}] \\ B_k(z_k) = A_k^+(z_{k+\frac{1}{2}}) \end{cases} \quad (9)$$

where $A_k^+(z_{k+\frac{1}{2}})$ represents the solution to problem (8) at half grid point $z_{k+\frac{1}{2}}$;

$$\begin{cases} \frac{\partial}{\partial z} A_k^-(z) = \mathcal{D} A_k^-(z) & \forall z \in [z_{k+\frac{1}{2}}, z_{k+1}] \\ A_k^-(z_{k+\frac{1}{2}}) = B_k(z_{k+1}) \end{cases} \quad (10)$$

where $B_k(z_{k+1})$ represents the solution to problem (9) at node z_{k+1} . An approximate solution to the NLSE (1) at grid node z_{k+1} is then given by $A_k^{[2]}(z_{k+1}) = A_k^-(z_{k+1})$. The principle of the Symmetric Split-Step scheme is depicted in figure 1. The most interesting thing of such a decomposition is that each one of the 3 problems (8), (9) and (10) can be solved much more easily than the NLSE (1) itself considered over the interval $[z_k, z_{k+1}]$. Moreover as detailed later (see proposition 2.1 p. 7) for h_k small enough $A_k^{[2]}(z_{k+1})$ provides an approximation of the solution to the NLSE (1) at grid point z_{k+1} . The exponent $^{[2]}$ in the notation of the approximate solution refers to the second order of accuracy of the Symmetric Split-Step method.

2.2. Solving the linear problems (8) and (10)

Problems (8) and (10) are in the form

$$\begin{cases} \frac{\partial}{\partial z} U(z) = \mathcal{D} U(z) & \forall z \in [a, b] \\ U(a) = \varphi \end{cases} \quad (11)$$

where $U(z)$ denotes the first partial function of the mapping $U : (z, t) \in [a, b] \times \mathbb{R} \mapsto U(z, t) \in \mathbb{C}$. It is known, see e.g. [11], that when the initial data φ is in $\mathbb{H}^N(\mathbb{R}, \mathbb{C})$, problem (11) has a unique

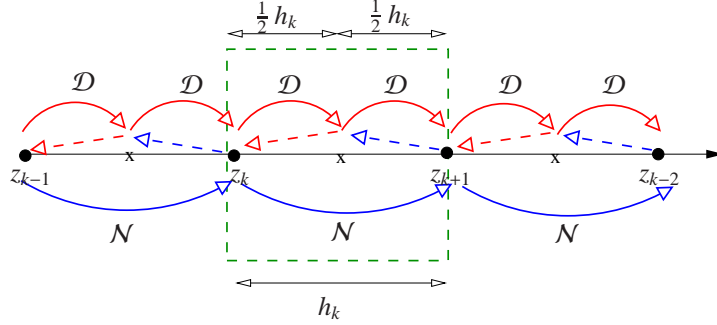


Figure 1: Principle of the Symmetric Split-Step scheme (computational step k is displayed in the dashed box).

solution $U : z \in [a, b] \mapsto U(z)$ belonging to $C^0([a, b]; \mathbb{H}^N(\mathbb{R}, \mathbb{C})) \cap C^1([a, b]; \mathbb{L}^2(\mathbb{R}, \mathbb{C}))$ which satisfies $\|U(z)\|_j = \|\varphi\|_j$ for all $j \in \{0, \dots, N\}$.

The solution to problem (11) can be computed by using the Fourier Transform (FT) approach. For a fixed value of the space variable z , we introduce the FT $\widehat{U}(z)$ of $U(z)$ with respect to the time variable t . We denote by \mathcal{F} the Fourier operator from $\mathbb{L}^2(\mathbb{R}, \mathbb{C})$ to $\mathbb{L}^2(\mathbb{R}, \mathbb{C})$ defined by continuous extension of the Fourier Transform definition for integrable functions and computed for all $u \in \mathbb{L}^2(\mathbb{R}, \mathbb{C})$ by an improper integral as

$$\forall \nu \in \mathbb{R} \quad \mathcal{F}(u)(\nu) = \widehat{u}(\nu) = \lim_{T \rightarrow +\infty} \int_{-T}^T u(t) e^{2i\nu t} dt.$$

We also denote by \mathcal{F}^{-1} the inverse Fourier Transform. From (11) we deduce that \widehat{U} satisfies

$$\begin{cases} \frac{\partial}{\partial z} \widehat{U}(z) &= \widehat{d}_\nu \widehat{U}(z) \quad \forall z \in [a, b] \\ \widehat{U}(a) &= \widehat{\varphi} \end{cases} \quad (12)$$

where $\widehat{d}_\nu = i \sum_{n=2}^N \frac{\beta_n}{n!} (2\pi\nu)^n$. The solution to the linear first order ODE problem (12) reads $\widehat{U}(z) = \widehat{\varphi} e^{\widehat{d}_\nu(z-a)}$. Therefore we have $U(b) = \mathcal{F}^{-1}[\widehat{U}(b)] = \mathcal{F}^{-1}[\widehat{\varphi} e^{\widehat{d}_\nu(b-a)}]$. As a consequence, the solution to problem (8) at grid point $z_{k+\frac{1}{2}}$ reads

$$A_k^+(z_{k+\frac{1}{2}}) = \mathcal{F}^{-1}[\widehat{A}_{k-1}(z_k) e^{\widehat{d}_\nu \frac{h_k}{2}}] \quad (13)$$

and the solution to problem (10) at grid point z_{k+1} reads

$$A_k^-(z_{k+1}) = \mathcal{F}^{-1}[\widehat{B}_k(z_{k+1}) e^{\widehat{d}_\nu \frac{h_k}{2}}]. \quad (14)$$

The Fourier transforms can be computed very efficiently by using the FFTW library [20] that supports a variety of algorithms and can choose the one it estimates or measures to be preferable in particular circumstances.

2.3. Solving the nonlinear problem

Since \mathcal{N} is locally Lipschitz continuous on $\mathbb{H}^m(\mathbb{R}, \mathbb{C})$ and continuous on $\mathbb{H}^m(\mathbb{R}, \mathbb{C})$, the Cauchy-Lipschitz theorem in Banach spaces gives the local existence of a unique maximal solution to the nonlinear ODE problem (9). The solution to problem (9) when \mathcal{N} is given by (6) can

be computed analytically. First, one can check that it admits the following integral representation form:

$$\forall z \in [z_k, z_{k+1}] \quad B_k(z) = A_k^+(z_{k+\frac{1}{2}}) \exp\left(-\frac{\alpha}{2}(z - z_k) + \int_{z_k}^z i\gamma |B_k(\zeta)|^2 d\zeta\right). \quad (15)$$

Multiplying each side of the ODE in (9) by $\overline{B_k(z)}$ (the complex conjugate of $B_k(z)$) and adding it to the complex conjugate equation deduced from (9) which has been previously multiplied by $B_k(z)$ shows that $\forall z \in [z_k, z_{k+1}]$

$$\frac{\partial}{\partial z} |B_k(z)|^2 = \overline{B_k(z)} \frac{\partial}{\partial z} B_k(z) + B_k(z) \frac{\partial}{\partial z} \overline{B_k(z)} = -\alpha |B_k(z)|^2. \quad (16)$$

We first consider the case when $\alpha = 0$. It turns out from (16) that the integrand in (15) is a constant function and we obtain

$$\forall z \in [z_k, z_{k+1}] \quad B_k(z) = A_k^+(z_{k+\frac{1}{2}}) \exp(i\gamma(z - z_k) |A_k^+(z_{k+\frac{1}{2}})|^2).$$

In the general case when $\alpha \neq 0$, it follows from (16) that for all $z \in [z_k, z_{k+1}]$ we have $|B_k(z)|^2 = |A_k^+(z_{k+\frac{1}{2}})|^2 e^{-\alpha(z-z_k)}$. Then, from (15) we deduce that for all $z \in [z_k, z_{k+1}]$

$$B_k(z) = A_k^+(z_{k+\frac{1}{2}}) \exp\left(-\frac{\alpha}{2}(z - z_k) - \frac{i\gamma}{\alpha} |A_k^+(z_{k+\frac{1}{2}})|^2 (e^{-\alpha(z-z_k)} - 1)\right).$$

Thus an analytical expression for the solution to the nonlinear problem (9) is known and in particular at grid point z_{k+1} we have

$$B_k(z_{k+1}) = \begin{cases} A_k^+(z_{k+\frac{1}{2}}) \exp(i\gamma h_k |A_k^+(z_{k+\frac{1}{2}})|^2) & \text{if } \alpha = 0 \\ A_k^+(z_{k+\frac{1}{2}}) \exp\left(-\frac{\alpha}{2} h_k - \frac{i\gamma}{\alpha} |A_k^+(z_{k+\frac{1}{2}})|^2 (e^{-\alpha h_k} - 1)\right) & \text{if } \alpha \neq 0 \end{cases}. \quad (17)$$

2.4. Error behavior for the Symmetric Split-Step scheme

The convergence of Split-Step methods applied to various forms of the Schrödinger equation is widely documented in the literature, see e.g. [21–23] where the authors prove that the convergence order of the Symmetric Split-Step method is 2. Namely, in the situation considered here the following result holds (see proposition 3.1 of [11]).

Proposition 2.1. *Let A denote the solution to the NLSE (1) and for all $k \in \{0, \dots, K-1\}$ let $A_k^{[2]}(z_{k+1})$ denote its approximation at grid point z_{k+1} computed by solving the 3 nested problems (8)–(9)–(10) with the initial condition $A_{k-1}^{[2]}(z_k) = A(z_k)$ assumed to be in $\mathbb{H}^{3N+1}(\mathbb{R}, \mathbb{C})$. Then, for h_k in a neighborhood of 0 we have the following estimate in $\mathbb{H}^1(\mathbb{R}, \mathbb{C})$:*

$$A(z_{k+1}) = A_k^{[2]}(z_{k+1}) + \mathcal{O}(h_k^3).$$

3. A truncated first order Split-Step scheme

3.1. First-order Lie-Trotter Split-Step scheme

As propound in [19], a local error estimate can be obtained by using the first order Lie-Trotter Split-Step scheme together with the Symmetric Split-Step one. The Lie-Trotter Split-Step

scheme is defined for all $k \in \{1, \dots, K-1\}$ by:

$$\begin{cases} \frac{\partial}{\partial z} A_k^*(z) = \mathcal{D} A_k^*(z) & \forall z \in [z_k, z_{k+1}] \\ A_k^*(z_k) = A_{k-1}^{[1]}(z_k) \end{cases} \quad (18)$$

where $A_{k-1}^{[1]}(z_k)$ represents the approximate solution at previous grid point z_k computed at step $k-1$; and

$$\begin{cases} \frac{\partial}{\partial z} B_k(z) = \mathcal{N}(B_k)(z) & \forall z \in [z_k, z_{k+1}] \\ B_k(z_k) = A_k^*(z_{k+1}) \end{cases} \quad (19)$$

where $A_k^*(z_{k+1})$ represents the solution to problem (18) at point z_{k+1} . The approximate solution to equation (1) at grid point z_{k+1} is then $A_k^{[1]}(z_{k+1}) = B_k(z_{k+1})$. The main drawback in using the Lie-Trotter Split-Step scheme is that the computations leading to the approximate solution cannot be factorized with the one of the Symmetric Split-Step scheme. The consequence is a significant extra cost for estimating the local error in this way, making the method not competitive when compared to the Step-Doubling method. In the next section we propose another first-order Split-Step scheme where most of the computations required for evaluating the first order approximate solution is also required for evaluating the Symmetric Split-Step approximate solution. The overall cost of this method for evaluating the local error is therefore very low.

3.2. The first-order Split-Step scheme

We consider the following Split-Step scheme defined for all $k \in \{1, \dots, K-1\}$ by:

$$\begin{cases} \frac{\partial}{\partial z} A_k^*(z) = \mathcal{D} A_k^*(z) & \forall z \in [z_k, z_{k+\frac{1}{2}}] \\ A_k^*(z_k) = A_{k-1}^{[1]}(z_k) \end{cases} \quad (20)$$

where $A_{k-1}^{[1]}(z_k)$ represents the approximate solution at previous grid point z_k computed at step $k-1$; and

$$\begin{cases} \frac{\partial}{\partial z} B_k(z) = \mathcal{N}(B_k)(z) & \forall z \in [z_k, z_{k+1}] \\ B_k(z_k) = A_k^*(z_{k+\frac{1}{2}}) \end{cases} \quad (21)$$

where $A_k^*(z_{k+\frac{1}{2}})$ represents the solution to problem (20) at half grid point $z_{k+\frac{1}{2}}$. The approximate solution to equation (1) at grid point z_{k+1} computed from the approximate solution $A_{k-1}^{[1]}(z_k)$ at grid point z_k is obtained by adding to $B_k(z_{k+1})$ a corrective term as follows:

$$A_k^{[1]}(z_{k+1}) = B_k(z_{k+1}) + \frac{1}{2} h_k \mathcal{D} A_{k-1}^{[1]}(z_k). \quad (22)$$

The exponent ^[1] in the notation of the approximate solution refers to the first order of accuracy of the method (this point is justified in the next section). The principle of this ‘‘truncated’’ Split-Step scheme is depicted in Fig. 2.

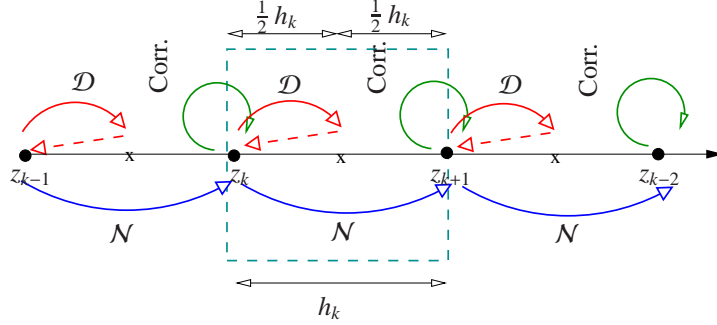


Figure 2: Principle of the "truncated" Split-Step scheme (computational step k is displayed in the dashed box).

3.3. Error analysis of the truncated Split-Step scheme

Since we are concerned by an analysis of the local error in the truncated Split-Step scheme defined by (20)–(21)–(22), we will assume in the following that at stage k for all $k \in \{0, \dots, K-1\}$, the initial data $A_{k-1}^{[1]}(z_k)$ is exact, i.e. $A_{k-1}^{[1]}(z_k) = A(z_{k-1})$ where A denotes the solution to equation (1).

Lemma 3.1. *For all $k \in \{0, \dots, K-1\}$, let A_k^* be the solution of problem (20) with the initial condition given by $A_k^*(z_k) = A(z_k)$ assumed to belong to $\mathbb{H}^{2N+1}(\mathbb{R}, \mathbb{C})$. For $h_k \in \mathbb{R}_+^*$ in a neighborhood of 0 we have the following equality in $\mathbb{H}^1(\mathbb{R}, \mathbb{C})$*

$$A_k^*(z_{k+\frac{1}{2}}) = A(z_k) + \frac{1}{2}h_k \mathcal{D}A(z_k) + \mathcal{O}(h_k^2).$$

Proof. A first order Taylor expansion for A_k^* between z_k and $z_{k+\frac{1}{2}}$ gives in $\mathbb{H}^1(\mathbb{R}, \mathbb{C})$

$$A_k^*(z_{k+\frac{1}{2}}) = A_k^*(z_k) + \frac{1}{2}h_k \frac{\partial}{\partial z} A_k^*(z_k) + \mathcal{O}(h_k^2).$$

Since A_k^* is solution to problem (20), we have $\frac{\partial}{\partial z} A_k^*(z_k) = \mathcal{D}A_k^*(z_k)$. Combining the 2 equalities gives the result under the assumption $A_k^*(z_k) = A(z_k)$. \square

Lemma 3.2. *For all $k \in \{0, \dots, K-1\}$, consider the 2 nested problems (20)–(21) with the initial condition for problem (20) given by $A_k^*(z_k) = A(z_k)$ assumed to belong to $\mathbb{H}^{2N+1}(\mathbb{R}, \mathbb{C})$. For $h_k \in \mathbb{R}_+^*$ in a neighborhood of 0, the solution B_k of problem (21) satisfies the following equality in $\mathbb{H}^1(\mathbb{R}, \mathbb{C})$:*

$$B_k(z_{k+1}) = A(z_{k+1}) - \frac{1}{2}h_k \mathcal{D}A(z_k) + \mathcal{O}(h_k^2).$$

Proof. A first order Taylor expansion applied to the solution B_k to problem (21) between z_k and z_{k+1} gives in $\mathbb{H}^1(\mathbb{R}, \mathbb{C})$:

$$\begin{aligned} B_k(z_{k+1}) &= B_k(z_k) + h_k \frac{\partial}{\partial z} B_k(z_k) + \mathcal{O}(h_k^2) = B_k(z_k) + h_k \mathcal{N}(B_k)(z_k) + \mathcal{O}(h_k^2) \\ &= A_k^*(z_{k+\frac{1}{2}}) + h_k \mathcal{N}(A_k^*)(z_{k+\frac{1}{2}}) + \mathcal{O}(h_k^2). \end{aligned}$$

Let us then consider a first order Taylor expansion of the solution to the NLSE (1) between z_k and z_{k+1} :

$$A(z_{k+1}) = A(z_k) + h_k \frac{\partial}{\partial z} A(z_k) + \mathcal{O}(h_k^2) = A(z_k) + h_k (\mathcal{D}A(z_k) + \mathcal{N}(A)(z_k)) + \mathcal{O}(h_k^2).$$

It follows that

$$\begin{aligned} A(z_{k+1}) - B_k(z_{k+1}) &= (A(z_k) - A_k^*(z_{k+\frac{1}{2}})) + h_k \mathcal{D}A(z_k) \\ &\quad + h_k (\mathcal{N}(A)(z_k) - \mathcal{N}(A_k^*)(z_{k+\frac{1}{2}})) + \mathcal{O}(h_k^2). \end{aligned} \quad (23)$$

Now consider a Taylor expansion of the operator \mathcal{N} between $A_k^*(z_{k+\frac{1}{2}})$ and $A(z_k)$:

$$\mathcal{N}(A)(z_k) - \mathcal{N}(A_k^*)(z_{k+\frac{1}{2}}) = \mathcal{N}'(A_k^*(z_{k+\frac{1}{2}}))(A(z_k) - A_k^*(z_{k+\frac{1}{2}})) + \mathcal{O}(\|A(z_k) - A_k^*(z_{k+\frac{1}{2}})\|_1^2).$$

From Lemma 3.1 we deduce that $\mathcal{N}(A)(z_k) - \mathcal{N}(A_k^*)(z_{k+\frac{1}{2}}) = \mathcal{O}(h_k)$ so that from (23)

$$A(z_{k+1}) - B_k(z_{k+1}) = (A(z_k) - A_k^*(z_{k+\frac{1}{2}})) + h_k \mathcal{D}A(z_k) + \mathcal{O}(h_k^2).$$

From Lemma 3.1 again, we conclude that $A(z_{k+1}) - B_k(z_{k+1}) = \frac{1}{2}h_k \mathcal{D}A(z_k) + \mathcal{O}(h_k^2)$. \square

From Lemmas 3.1 and 3.2 we finally deduce the following result which states that the Split-Step scheme (20)–(21)–(22) is first order accurate.

Proposition 3.3. *Let A denote the solution to the NLSE (1) under the initial condition $A(0) = a_0$ at $z = 0$ where a_0 is a given function in $\mathbb{H}^{2N+1}(\mathbb{R}, \mathbb{C})$. For all $k \in \{0, \dots, K-1\}$, let $A_k^{[1]}(z_{k+1})$ be the function given by relation (22) where $B_k(z_{k+1})$ is the solution at grid point z_{k+1} of the 2 nested problems (20)–(21) under the initial condition for problem (20) given by $A_k^*(z_k) = A(z_k)$. For $h_k \in \mathbb{R}_+^*$ in a neighborhood of 0 we have the following equality in $\mathbb{H}^1(\mathbb{R}, \mathbb{C})$:*

$$A(z_{k+1}) = A_k^{[1]}(z_{k+1}) + \mathcal{O}(h_k^2).$$

Remark A first order Taylor expansion of the solution to problem (10) between $z_{k+\frac{1}{2}}$ and z_{k+1} gives

$$A_k^-(z_{k+1}) = A_k^-(z_{k+\frac{1}{2}}) + \frac{h_k}{2} \frac{\partial}{\partial z} A_k^-(z_{k+\frac{1}{2}}) + \mathcal{O}(h_k^2) = B_k(z_{k+1}) + \frac{h_k}{2} \frac{\partial}{\partial z} B_k(z_{k+1}) + \mathcal{O}(h_k^2)$$

and from lemma 3.2 we deduce that

$$A_k^{[1]}(z_{k+1}) = A_k^-(z_{k+1}) = B_k(z_{k+1}) + \frac{h_k}{2} \frac{\partial}{\partial z} A_{k-1}^{[1]}(z_k) + \mathcal{O}(h_k^2).$$

Therefore the corrective term (22) is nothing but a first order Taylor expansion of the solution to problem (10). A similar first order Taylor expansion could be considered instead of solving problem (8) with a resulting approximation scheme having the same order of accuracy, but the resulting computational procedure would not be anymore fully embedded in the Symmetric Split-Step one, resulting in an increase of the computational cost.

4. The Embedded Split-Step method with adaptive step-size control

4.1. Numerical approximation of the local error for the Split-Step scheme

Assuming that the solution value at grid point z_k is regarded as exact (because we are concerned by an estimation of the local error), we denote by $A_k^{[1]}$ (resp. $A_k^{[2]}$) the approximate solution computed at the current grid point z_k by the first order (resp. the second order) above Split-Step scheme. From propositions 2.1 and 3.3 we deduce that for a regular enough initial condition, the local error at grid point z_{k+1} for each of the 2 schemes is respectively given, for h_k in a neighborhood of 0 and $\forall t \in \mathbb{R}$, by

$$\ell_{k+1}^{[1]}(t) = A(z_{k+1}, t) - A_k^{[1]}(z_{k+1}, t) = C_{1,k} h_k^2 + \mathcal{O}(h_k^3) \quad (24)$$

$$\ell_{k+1}^{[2]}(t) = A(z_{k+1}, t) - A_k^{[2]}(z_{k+1}, t) = C_{2,k} h_k^3 + \mathcal{O}(h_k^4) \quad (25)$$

where $C_{1,k}$ and $C_{2,k}$ denote 2 numbers independent of h_k . By taking the difference between these 2 relations we obtain: $\forall t \in \mathbb{R}$

$$A_k^{[2]}(z_{k+1}, t) - A_k^{[1]}(z_{k+1}, t) = C_{1,k} h_k^2 + \mathcal{O}(h_k^3).$$

Thus the local error for the first order Split-Step scheme at grid point z_{k+1} can be approximated, with an error in $\mathcal{O}(h_k^3)$, in the following way: $\forall t \in \mathbb{R}$

$$\ell_{k+1}^{[1]}(t) \approx C_{1,k} h_k^2 \approx A_k^{[2]}(z_{k+1}, t) - A_k^{[1]}(z_{k+1}, t). \quad (26)$$

Performing integration over t in \mathbb{R} , we obtain the following approximation for the \mathbb{L}^2 -local error at grid point z_{k+1}

$$\|\ell_{k+1}^{[1]}\|_0 \approx \left(\int_{\mathbb{R}} |A_k^{[2]}(z_{k+1}, t) - A_k^{[1]}(z_{k+1}, t)|^2 dt \right)^{\frac{1}{2}} \approx \sqrt{h_t} \left(\sum_{j=0}^{J-1} |A_{k+1}^{[2]}(t_j) - A_{k+1}^{[1]}(t_j)|^2 \right)^{\frac{1}{2}} \quad (27)$$

where, for simplicity, the last approximation results from the use of the rectangle quadrature rule over a discretization $(t_j)_{j=0, \dots, J}$ with a constant step-size h_t of the interval of observation. Note that the trapezoidal quadrature rule could also be used and would provide a more accurate result for the same cost.

We have to point out that relation (26) gives an approximation of the local error corresponding to the solution computed with the first order Split-Step method and consequently the size of the steps delivered by the adaptive step-size control method will be optimal for the first order Split-Step scheme. However, the solution computed by the Symmetric Split-Step method is a better approximation than the one computed by the first order Split-Step method and it is thus kept as the approximate solution. This is very common in such a situation and it is referred to as "local extrapolation".

4.2. The Embedded Split-Step method

The computational sequence for one step of the Embedded Split-Step method can be understood as follows. For $k \in \mathbb{N}$, let $u_{k+1}^{[1]}$ denotes the solution at grid point z_{k+1} computed by the first order Split-Step scheme defined at step k by (20)–(21)–(22) and let $u_{k+1}^{[2]}$ denotes the solution at grid point z_{k+1} computed by the Symmetric Split-Step method defined at step k by (8)–(9)–(10). As mentioned before, the solution computed by the Symmetric Split-Step scheme is a better

approximation than the one computed by the first order Split-Step scheme and it is kept as the approximate solution at each grid point. As a consequence, the initial condition in (8) and (20) is $A_{k-1}^{[2]}(z_k)$ and the 2 linear PDE problems are actually identical. It follows that the 2 problems (9) and (21) are also identical and the 2 Split-Step schemes only differ by (10) and (22).

The way $u_{k+1}^{[1]}$ and $u_{k+1}^{[2]}$ are obtained from $u_k^{[2]}$ (or actually their Fourier Transforms $\widehat{u}_{k+1}^{[1]}$ and $\widehat{u}_{k+1}^{[2]}$ from $\widehat{u}_k^{[2]}$) as well as the way the local error is estimated, can be summarized by the following computational sequence:

$$\widehat{v}_{\frac{1}{2}} = \exp\left(\frac{h_k}{2}\widehat{d}_v\right) \times \widehat{u}_k^{[2]} \quad \text{where } \widehat{d}_v \text{ is defined in (12)}$$

$$v_{\frac{1}{2}} = \mathcal{F}^{-1}(\widehat{v}_{\frac{1}{2}})$$

$$v_1 = \begin{cases} v_{\frac{1}{2}} \exp\left(-\frac{\alpha}{2}h_k - i\gamma|v_{\frac{1}{2}}|^2 \frac{e^{\alpha h_k} - 1}{\alpha}\right) & \text{if } \alpha \neq 0 \\ v_{\frac{1}{2}} \exp\left(i\gamma h_k |v_{\frac{1}{2}}|^2\right) & \text{if } \alpha = 0 \end{cases}$$

$$\widehat{v}_1 = \mathcal{F}(v_1)$$

$$\widehat{u}_{k+1}^{[2]} = \exp\left(\frac{h_k}{2}\widehat{d}_v\right) \times \widehat{v}_1$$

$$\widehat{u}_{k+1}^{[1]} = \widehat{v}_1 + \frac{h_k}{2}\widehat{d}_v \times \widehat{u}_k^{[2]}$$

$$\text{local error} = \|\widehat{u}_{k+1}^{[2]} - \widehat{u}_{k+1}^{[1]}\|_0 \quad (\text{from Parseval's theorem})$$

$$\text{relative local error} = \|\widehat{u}_{k+1}^{[2]} - \widehat{u}_{k+1}^{[1]}\|_0 / \|\widehat{u}_{k+1}^{[2]}\|_0$$

When compared to the standard version of the Symmetric Split-Step method, the over-cost of the above computational procedure for delivering the local error estimate reduces to the computation of the term $\widehat{u}_{k+1}^{[1]}$. Since the value of $\frac{h_k}{2}\widehat{d}_v$ is required when implementing the Symmetric Split-Step scheme, the over-cost at each step is 1 multiplication and 1 addition times the number of sampling points in the frequency domain.

4.3. Step-size control

For step-size control, a tolerance “tol” is given as bound on the local error estimate. A step-size control strategy consists in rejecting the current step-size if it gives an estimated local error “err” higher than the specified tolerance and in accepting the solution computed with this step-size if otherwise. When the current step-size is rejected, a new smaller step-size has to be chosen to recompute the solution from the current grid point. On the contrary, when the current step-size meets the tolerance requirement for the local error, it has to be scaled up for the next computation step. We consider the Symmetric Split-step method and the Split-Step method defined respectively by (8)–(9)–(10) and (20)–(21)–(22), and we assume that the leading term in the asymptotic expansion (24) of the local error dominates the others for the current value of the step-size h_k . From (24) and (27) there exists $C \in \mathbb{R}^+$ such that $\|\ell_{k+1}^{[1]}\|_0 = C h_k^2$. The optimal step-size h_{opt} is the one for which the local error estimate is the closest to the prescribed tolerance tol, i.e. $C h_{\text{opt}}^2 = \text{tol}$. By eliminating the constant C from these 2 relations we obtain

$$h_{\text{opt}} = h_k \sqrt{\frac{\text{tol}}{\text{err}}}.$$

where $\text{err} = \|\ell_{k+1}^{[1]}\|_0$. In the previous relationship it is common to consider an estimate for the relative local error and a relative tolerance “tol”. It is the choice we adopt in the following.

For robustness the step-size control has to be designed in order to respond as smoothly as possible with real or apparent abrupt changes in behavior. That is the reason why it is imposed that the new step-size does not exceed α_1 times the current step-size above and α_2 times the current step-size below. In order to avoid situations where the specified tolerance is ever exceeded resulting in rejecting too many steps, a safety factor is introduced: if h_{opt} is the value of the step-size estimated to give a predicted truncation error equal to the tolerance, then the smaller value $\alpha_3 h_{\text{opt}}$ is used instead. Following these requirements, the following step-size control formula is considered

$$h_{\text{new}} = \max \left(\alpha_2, \min \left(\alpha_1, \alpha_3 \sqrt{\frac{\text{tol}}{\|\text{err}\|}} \right) \right) h_k \quad (28)$$

where tol denotes the relative tolerance value specified by the user as a bound on the relative local error estimated by (27). Suggested constant values for α_1 , α_2 and α_3 are respectively 2.0, 0.5 and 0.9.

4.4. Algorithm for the Embedded Split-Step method

ESS algorithm

Require: Array u containing the input pulse envelope sampled over the time interval

Array $[t_j]_{j=1,\dots,J}$ containing the time sampling points

Array $[v_j]_{j=1,\dots,J}$ containing the frequency sampling points

Initial step-size h and tolerance tol

Ensure: Array $[z_k]_{k=0,\dots,K}$ containing the spatial grid points

Array u containing the output pulse envelope sampled over the time interval at the fiber end

```

1: {Initializations}
2: for  $j = 1, \dots, J$  do
3:    $\widehat{d}[j] \leftarrow i \sum_{n=2}^N \frac{\beta_n}{n!} (2\pi v_j)^n$ 
4: end for
5:  $k = 0; z[0] = 0$ 
6:  $\widehat{u}^{[2]} \leftarrow \text{FFT}(u, \text{forward})$ 
7: {Loop over the propagation subinterval}
8: while  $z[k] \leq L$  do
9:   {Solving the first linear problem}
10:  for  $j = 1, \dots, J$  do
11:     $tfexpd[j] \leftarrow \exp(\frac{h}{2}\widehat{d}[j])$ 
12:     $\widehat{u}_{\frac{1}{2}}[j] \leftarrow tfexpd[j] \times \widehat{u}^{[2]}[j]$ 
13:  end for
14:   $u_{\frac{1}{2}} \leftarrow \text{FFT}(\widehat{u}_{\frac{1}{2}}, \text{backward})$ 
15:  {Solving the nonlinear problem}
16:  if  $\alpha \neq 0$  then
17:    for  $j = 1, \dots, J$  do
18:       $u_1[j] \leftarrow u_{\frac{1}{2}}[j] \times \exp(-\frac{1}{2}\alpha h - \frac{i\gamma}{\alpha}(e^{\alpha h} - 1)|u_{\frac{1}{2}}[j]|^2)$ 
19:    end for
20:  else
21:    for  $j = 1, \dots, J$  do
22:       $u_1[j] \leftarrow u_{\frac{1}{2}}[j] \times \exp(i\gamma h|u_{\frac{1}{2}}[j]|^2)$ 
23:    end for

```

```

24: end if
25:  $\widehat{u}_1 \leftarrow \text{FFT}(u_1, \text{forward})$ 
26: {Compute the 2 approximate solutions}
27: for  $j = 1, \dots, J$  do
28:    $\widehat{u}_2^{[1]}[j] \leftarrow \widehat{u}_1[j] + \frac{h}{2} \widehat{d}[j] \widehat{u}^{[2]}[j]$  {First order approximate solution}
29:    $\widehat{u}_2^{[2]}[j] \leftarrow \text{tfexpd}[j] \times \widehat{u}_1[j]$  {Second order approximate solution}
30: end for
31: {Step-size control}
32:  $\text{err} \leftarrow 0$ 
33:  $\text{norm\_sol} \leftarrow 0$ 
34: for  $j = 1, \dots, J$  do
35:    $\text{norm\_sol} \leftarrow \text{norm\_sol} + |\widehat{u}_2^{[2]}[j]|^2$ 
36:    $\text{err} \leftarrow \text{err} + |\widehat{u}_2^{[2]}[j] - \widehat{u}_2^{[1]}[j]|^2$ 
37: end for
38:  $\text{err} \leftarrow \sqrt{\text{err}/\text{norm\_sol}}$ 
39:  $h_{\text{opt}} = \max\left(0.5, \min\left(2.0, 0.9 \sqrt{\frac{\text{tol}}{\text{err}}}\right)\right)h$  {Optimal step-size for the given prescribed tolerance}
40: if  $\text{err} \leq \text{tol}$  then
41:   {The current local error matches the tolerance}
42:    $z[k+1] = z[k] + h$  {New grid point is confirmed}
43:    $h = \min(h_{\text{opt}}, L - z[k+1])$  {New step-size value}
44:    $\widehat{u}^{[2]} \leftarrow \widehat{u}_2^{[2]}$  {Initial condition for the next step computations}
45:    $k \leftarrow k + 1$ 
46:   {The following line can be removed when only the solution at the fiber end is required and placed after the end of while loop}
47:    $u \leftarrow \text{FFT}(\widehat{u}^{[2]}, \text{backward})$  {Array  $u$  contains the time sampled values  $[A_k(z_{k+1}, t_j)]_{j=1, \dots, J}$  of the signal amplitude at grid point  $z_{k+1}$ }
48: else
49:   {The current local error does not match the tolerance}
50:    $h = h_{\text{opt}}$  {New computation from  $z_k$  with smaller step-size  $h_{\text{opt}}$  is necessary}
51: end if
52: end while

```

$\text{FFT}(u, \text{forward})$ stands for a call to the Fast Fourier Transform (FFT) algorithm to compute the Discrete Fourier Transform (DFT) of array u , $\text{FFT}(u, \text{backward})$ stands for a call to FFT algorithm to compute the inverse DFT of array u ,

5. Numerical comparisons on benchmark problems in optics

5.1. The Symmetric Split-Step method with local error estimate by Step-Doubling

The idea behind the Step-Doubling method for estimation of the local error (widely used for adaptive step-size control in quadrature methods for integral or ODE [15, 17]) is the following: the local error $\ell_{k+1}^{[2]}$ for the Symmetric Split-Step method at grid point z_{k+1} given by (25) reads

$$\ell_{k+1}^{[2]} = A(z_{k+1}) - A_k^{[2]}(z_{k+1}) = C_{2,k} h_k^3 + \mathcal{O}(h_k^4) \quad (29)$$

where A denotes the exact solution to the NLSE (1), $A_k^{[2]}$ denotes the approximate solution computed by the Symmetric Split-Step method and $C_{2,k}$ denotes a positive number independent of h_k . Let $u_{k+1}^{[2]}$ be the solution at grid point z_{k+1} computed from grid point z_k by the Symmetric Split-Step method using one step of size h_k , and let $v_{k+1}^{[2]}$ be the solution computed using two steps of size $h_k/2$, in both cases assuming the solution at grid point z_k to be exact (since we are interested in the local error). Additionally the following assumption is made: (\mathcal{H}) “the local error after 2 half steps is twice the local error after one half step” (which consists in an approximation since the initial data for the second half-step is actually the approximated solution computed after the first half-step and not the exact one; such an approximation is relevant here). Then, from (29) we deduce that

$$A(z_{k+1}) - u_{k+1}^{[2]} = C_{2,k} h_k^3 + \mathcal{O}(h_k^4) \quad \text{and} \quad A(z_{k+1}) - v_{k+1}^{[2]} = 2 C_{2,k} \left(\frac{h_k}{2}\right)^3 + \mathcal{O}(h_k^4)$$

and therefore by difference between these 2 relations we get $v_{k+1}^{[2]} - u_{k+1}^{[2]} = \frac{3}{4} C_{2,k} h_k^3 + \mathcal{O}(h_k^4)$. Thus the local error related to the Symmetric Split-Step scheme at grid point z_{k+1} can be approximated, with an error in $\mathcal{O}(h_k^4)$, by

$$\ell_{k+1}^{[2]} \approx C_{2,k} h_k^3 \approx \frac{4}{3} (v_{k+1}^{[2]} - u_{k+1}^{[2]}). \quad (30)$$

We have to point out that relation (30) gives an approximation of the local error corresponding to the solution $u_{k+1}^{[2]}$ computed by the Symmetric Split-Step scheme over the coarse grid with step-size h_k . However the fine mesh grid solution $v_{k+1}^{[2]}$ is a better approximation and in practice it is kept as the approximate solution and propagated along the fiber. This process is referred in the literature as the “local extrapolation mode”. The over-cost of estimating the local error in this way is the cost of the computation of the coarse mesh grid solution and this cost is approximately half the cost of the computation of the fine mesh grid solution since the step-size is twice as large. Thus, estimating the local error using the step doubling approach is liable of an extra computational cost of 50% more than the cost of the computation of the approximated solution itself.

5.2. Soliton propagation

When $\alpha = 0$ and $\beta_2 < 0$, the NLSE (1) admits an exact solution known as the optical soliton [1, 2]. Namely, if the source term is given by $a_0 : t \mapsto N_s / (\sqrt{\gamma L_D} \text{ch}(t/T_0))$ where N_s is the soliton order, T_0 is the pulse half-width and $L_D = -T_0^2/\beta_2$ is the dispersion length, then the solution to the NLSE at the soliton period $z_p = \frac{\pi}{2} L_D$ is given by

$$\forall t \in \mathbb{R} \quad A(z, t) = \frac{N_s}{\sqrt{\gamma L_D}} \frac{e^{izN_s^2/(2L_D)}}{\text{ch}(t/T_0)}. \quad (31)$$

We have first considered a 3rd order soliton ($N_s = 3$) with the following physical parameters for the numerical experiment: $L = \frac{\pi}{2} L_D = 19.80$ m, $\lambda = 1550$ nm, $\gamma = 4.3 \text{ W}^{-1} \text{ km}^{-1}$, $\beta_2 = -19.83 \text{ ps}^2 \text{ km}^{-1}$, $T_0 = 0.5$ ps. For these experimental values, the self-phase modulation (SPM) is preeminent and it gives rise to an intensity dependent phase shift and induces a spectral broadening which increases with the propagation distance z , see e.g. [1]. It is therefore mandatory to have a number of sampling points for the FFT computations large enough to embrace all the spectrum at any propagation distance. Here it was set to 2^{18} . The initial step-size was set to 0.1 m. Computations were done on a AMD A8 Personal Computer.

Method	Tol.	CPU (s.)	Nb FFT	Nb steps (reject.)	Quad. Err.	Sup. Err.
E3S	10^{-3}	172	834	416 (2)	0.0044726	0.004526
	10^{-4}	531	2618	1308 (1)	0.0010064	0.0014015
SD	10^{-3}	182	1016	169 (18) / 338 (36)	0.011662	0.012961
	10^{-4}	350	1922	320 (0) / 640 (0)	0.0020821	0.0022514

Table 1: Comparison of the Embedded Symmetric Split-Step (E3S) and the Symmetric Split-Step with Step-Doubling (SD) methods for solving the NLSE for a 3rd order Soliton. For the Step-Doubling method we have indicated the number of steps for both the coarse and fine grids.

For comparison purposes we have summarized in Table 1 the main features of both the Embedded Symmetric Split-Step (E3S) method and the Symmetric Split-Step with Step-Doubling (SD) method when applied for solving the normalized NLSE (3) with the above physical parameter values. We provide the CPU time in second, the number of FFT achieved, the number of computational steps with inside the brackets the number of steps rejected by the adaptive step-size control strategy and the quadratic relative error and the maximum relative error at the fiber end for tolerance values of 10^{-3} and 10^{-4} . For a tolerance set to 10^{-3} , one can observe that the E3S method requires a much larger number of computational steps (416) than the SD method (169) but provides a result 2.5 times more accurate for a very close computation time. Similar comments can be done in the case when the tolerance was set to 10^{-4} (even if in this latter case the CPU time for the E3S method is 1.5 time larger than the CPU time required by the SD method). In this example, the E3S method selects smaller step-sizes (average size of 0.0478 m for a tolerance 10^{-3}) than the SD method (average size of 0.1311 m or actually 0.0655 m since it is the fine grid solution which is propagated). This behavior is confirmed in Fig. 3 where the evolution of the step-size along the fiber for the 2 methods is represented. This can be understood as follows. The adaptive step-size strategy in the E3S method estimates the local error for the embedded 1st order Split-Step scheme. This error is likely to be higher than the actual local error corresponding to the propagation of the solution of the 2nd order Symmetric Split-Step scheme. This local error is more accurately estimated by the Step-Doubling method. The local error in the E3S method is therefore overestimated resulting in a selection of step-sizes smaller than actually required. This is the reason why the E3S method should not be used for too small tolerance values. However, the E3S method counterbalances this drawback by requiring 3 times less FFT evaluations per step and we can observe a gain in the computation time. Indeed, in order to obtain at the fiber end the same relative quadratic error of 0.45% corresponding to a tolerance 10^{-3} for the E3S method, the SD method should be used with a tolerance of $2.5 \cdot 10^{-4}$. The CPU time is 172 s for the E3S method versus 258 s for the SD method which represents an difference of approximately 50%. One can infer that whenever the number of FFT nodes will be larger than 2^{18} the E3S method will be even more efficient than the SD method (since the cost of each FFT will increase). On the contrary, when FFT can be computed at a lower cost (i.e. when the required number of FFT nodes is lower than 2^{18}), the SD method will be more efficient. This is confirmed by additional simulations: for instance when the number of FFT nodes is set to 2^{20} we obtain a CPU time of 676 s for the E3S method versus 1065 s for the SD method for a relative quadratic error of 0.45% at the fiber end and the same physical values as before. We refer to [24] for a practical application in optics requiring up to 2^{23} FFT nodes.

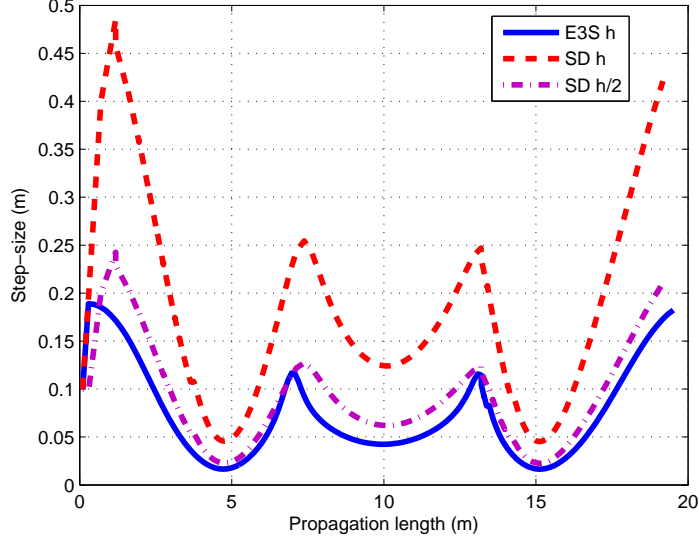


Figure 3: Evolution of the step-size along the fiber for the E3S and the SD methods (considered here over the coarse and the fine grids) when solving the NLSE for a 3rd order soliton with a tolerance set to 10^{-3} .

5.3. Soliton collisions

We present in this section numerical simulation results for the collision of 2 first order solitons [1]. It is known that when two neighboring solitons are launched with the same phase, they are initially attracted towards each other and then the two pulses periodically coalesce to form one pulse and separate [25]. The source term was

$$a_0 : t \in \mathbb{R} \mapsto \frac{1}{\sqrt{\gamma L_D}} \left(\frac{1}{\text{ch}((t - T_1)/T_0)} + \frac{Re^{i\phi}}{\text{ch}(R(t + T_1)/T_0)} \right)$$

where T_0 is the pulse half-width, $L_D = -T_0^2/\beta_2$ is the dispersion length, R accounts for the relative amplitude, ϕ for the relative phase shift and T_1 for the initial separation time. The following physical parameters were taken for the numerical experiment: $L = 5000$ km, $\lambda = 1550$ nm, $\gamma = 2.2 \text{ W}^{-1} \text{ km}^{-1}$, $\beta_2 = -0.1 \text{ ps}^2 \text{ km}^{-1}$, $T_0 = 4$ ps, $T_1 = 100$ ps, $R = 1$ and $\phi = 0$. With these numerical values, the collision of the 2 solitons is predicted to happen at a distance of 4161 km [1]. The simulation time windows was 400 ps and the number of FFT nodes was 2^{14} . The initial step-size was set to 1 km and the tolerance to 10^{-3} .

For comparison purposes we have summarized in Table 1 the main features of the Embedded Symmetric Split-Step (E3S) method and of the Symmetric Split-Step with Step-Doubling (SD) method when applied for solving the NLSE with the above physical parameter values. We provide the CPU time in seconds, the number of FFT achieved and the number of computational steps. Inside the brackets are the number of steps rejected by the adaptive step-size control strategy. The global error at the fiber end has been computed by comparison to a reference solution obtained with a constant step-size of 0.1 km. Fig. 4 depicts the evolution of the step-size along the fiber for the E3S and the SD methods (considered here over the coarse and the fine grids). The same observations made in the previous example are also valid here.

Method	CPU time (s.)	Nb FFT	Nb steps (rejected)	Quad. Err.	Sup. Err.
E3S	12.2	974	486 (4)	0.014715	0.014978
SD	11.6	1064	177 (16) / 354 (32)	0.031737	0.032481

Table 2: Comparison of the Embedded Symmetric Split-Step (E3S) and the Symmetric Split-Step with Step-Doubling (SD) methods for solving the NLSE for soliton collision for a tolerance set to 10^{-3} . For the Step-Doubling method we have indicated the number of steps for both the coarse and fine grids.

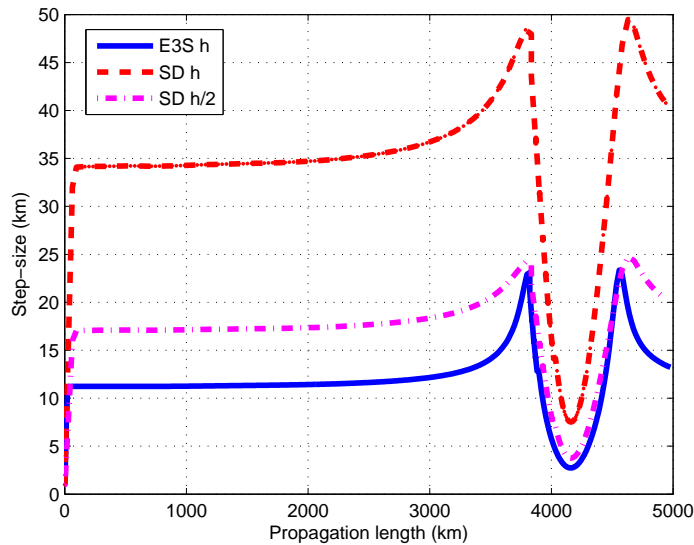


Figure 4: Evolution of the step-size along the fiber for the E3S and the SD methods (considered here over the coarse and the fine grids) when solving the NLSE for soliton collision for a tolerance set to 10^{-3} .

In order to obtain at the fiber end the same relative quadratic error of 1.47% corresponding to a tolerance 10^{-3} for the E3S method, the SD method should be used with a tolerance of $3 \cdot 10^{-4}$. The CPU time for the E3S method is then 17.0 s and 256 steps are required.

6. Conclusion

We have presented a way of estimating the local error for adaptive step-size control purposes when solving the nonlinear Schrödinger equation (NLSE) by using the Symmetric Split-Step method. Compared to the "step-doubling" approach where the 2 approximated solutions are obtained by solving the NLSE by the Symmetric Split-Step method with 2 different step-size (the finest one being half the coarse one) resulting in a computational over-cost of 50%. Our approach gives a coarse approximated solution at low cost by a first order Split-Step scheme designed to be embedded into the Symmetric Split-Step method. The numerical investigations we have conducted show that this way of estimating the local error for adaptive step-size purposes is valuable compared to the "step-doubling" approach when the computational cost of the Fourier Transform is significant (which is likely to occur in optics e.g. when the self-phase modulation

induces a large spectral broadening) since the "step-doubling" approach increases by a factor 3 the number of Fourier Transforms to be achieved compared to the Symmetric Split-Step method without adaptive step-size control. The main drawback of the proposed approach is that since the local error for the Symmetric Split-Step method is estimated from a first order Split-Step scheme, it is overestimated resulting in a selection of step-sizes smaller than optimal. The various parameter in the step-size selection formula could however be empirically tuned to take into account this particularity. Alternatively higher order embedded Split-Step scheme could be used.

The approach presented in this paper is not only applicable to the NLSE but to any evolution type PDE for which a solution can be computed by the Symmetric Split-Step method with an explicit solution for the nonlinear ODE problem (9) or with a solution for the nonlinear ODE problem (9) obtained by a numerical method with an order of accuracy much higher than that of the Symmetric Split-Step method.

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