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Microlocal approach towards construction of nonreflecting boundary conditions

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ABSTRACT

This paper addresses the problem of construction of non-reflecting boundary condition for certain second-order nonlinear dispersive equations. It is shown that using the concept of microlocality it is possible to relax the requirement of compact support of the initial data. The method is demonstrated for a class of initial data such that outside the computational domain it behaves like a continuous-wave. The generalization is detailed for two existing schemes in the framework of pseudo-differential calculus, namely, Szeftel's method (Szeftel (2006) [1]) and gauge transformation strategy (Antoine et al. (2006) [2]). Efficient numerical implementation is discussed and a comparative performance analysis is presented. The paper also briefly surveys the possibility of extension of the method to higher-dimensional PDEs.

1. Introduction

This paper focuses on the methods of constructing non-reflecting boundary conditions for numerical solution of certain second-order nonlinear dispersive equations for a special class of initial conditions that behave like continuous wave (CW) background outside a certain compact domain. Such problems arise in the context of dispersive systems in various areas of physics like fluid mechanics, nonlinear optics, plasma physics and quantum mechanics. In nonlinear optics, propagation of light in fibers is governed by the nonlinear Schrödinger equation and its various generalizations [3–5]. A CW background arises in these systems as the steady state solution. The study of such solutions is important on account of their application in coherent optical transmission which uses amplitude- and/or phase-modulated quasi-CW signals. In particular, evolution of modulational instabilities (MI) over CW background has been a subject of extensive study [6–9]. Other physically interesting solutions which exhibit such a non-vanishing behavior are Bright solitons on CW background [4,10–13] and Dark/Gray solitons [4,14,15] solutions. In quantum mechanics, the nonlinear Schrödinger equation with a time varying potential describes the evolution of Bose–Einstein condensates in the one dimensional limit of the Gross–Pitaevskii equation [16,17]. Such systems also posses soliton-like solutions which behave like CW background outside a bounded interval.

In numerical solution of such evolution problems which are formulated on an unbounded domain, the truncation to a bounded domain poses an additional problem of choosing the right kind of boundary conditions at the fictitious boundaries. Solution to this problem for different evolution PDEs, for instance, linear and nonlinear evolution PDEs in $\mathbb{R}$, in the current research literature can be found under the caption *transparent boundary conditions*, *artificial boundary conditions* and *absorbing*

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boundary conditions [2,18–22]. Transparent boundary conditions are exact, in that the truncated initial boundary value problem (IBVP) is completely identical to the original evolution problem posed on an unbounded domain; however, there are no general schemes for the construction of these conditions for an arbitrary PDE on account of the requirement of integrability. Further, such conditions prove to be prohibitively complex for implementation in most cases; therefore, the current interest in this field is diverted to the construction of efficient approximations of the exact transparent boundary operators. The latter two of the listed above belong to this class of boundary conditions. While all of these approximate methods tend to reduce unphysical reflections, there are some subtle differences in their properties and limitations. A rigorous justification for all such approximation techniques exist only for linear problems, however, we find various heuristic ideas successfully implemented for nonlinear problems as well. Among many of such strategies (for instance, perfectly matched layer approach [23,24], method of time-splitting [25]) is the *pseudo-differential approach* which first appeared in the context of hyperbolic wave equations with variable coefficients [26,27]; we refer to such conditions as *artificial boundary conditions* (ABCs) which are derived as approximations of some pseudo-differential operator. Pseudo-differential operators [28–30] are a generalization of differential operators and most of the transparent boundary operators, specially for evolution PDEs in $\mathbb{R}$, happen to be of this kind (at least up to a smoothing operator), consequently, this approach provides a somewhat general scheme for the solution of the boundary condition problem for arbitrary PDEs irrespective of their integrability.

The pseudo-differential approach, in the way it is applied, gives the asymptotic form of the transparent boundary operators valid for small time durations or high-frequency (refers to the temporal frequency) components of the evolving profile [2]. This paper adopts the pseudo-differential approach and the concept of microlocalization towards designing these novel boundary conditions. In particular, the two basic ideas that have been exploited in this work are: the possibility of obtaining a *Nirenberg-type factorization* [29] and the construction of *microparametrices* [30,31]. While the former scheme already exists in the literature, the latter, to the best of my knowledge, is a new technique applied in this paper to achieve a greater generalization towards construction of artificial boundary conditions.

For practical reasons, the class of initial conditions for which ABCs can be obtained is very limited as it is mandatory to impose a certain behavior on the initial condition outside the computational domain. This paper mostly considers how to relax conditions such as the requirement of compact support of the initial data. From a physical point of view, it is interesting to see how the existing results can be generalized for the class of initial data which behaves like a continuous-wave (CW) outside the computational domain. The method developed in this paper is demonstrated by treating the Schrödinger equation with possible nonlinearity and a variable potential. In particular we compare two known strategies of applying the pseudo-differential approach, both of which are first generalized in the unified way. The two methods are: (1) Szeftel's [1] method and (2) gauge transformation strategy [2]. Efficient numerical implementation is discussed and a complete error analysis is presented using known analytical solutions of the equation being considered.

There is a considerable amount of interest in methods which allow generalization to higher-dimensional PDEs. This motivates a brief survey of possibilities of extension of our method to the higher dimensions which is presented in Section 6.[1] A complete account of this generalization will be published elsewhere.

2. Preliminary discussion

Let us consider the evolution problem of the following form

$$\begin{aligned}
&i\partial_t u + \partial_x^2 u + \phi(u,x,t)u = 0 \quad (x,t) \in \mathbb{R}\times\mathbb{R}_+,\\
&u(x,0) = u_0(x),\\
&\lim_{|x|\to\infty} \bigl|u(x,t)\bigr| < M, \quad t>0.
\end{aligned} \tag{1}$$

Here, we would like to consider a larger class of initial conditions, $u_0(x) \in \mathcal{C}^\infty(\mathbb{R})$,[2] such that outside a compact domain, say $\overline{\Omega}_i$, $u_0(x) = A_{l,r}e^{i\kappa_{l,r}x}$ for $x \in \Omega_{l,r}$, respectively, where $A_{l,r}$, $\kappa_{l,r}$ are constants. The domain Ω_i can be taken as the computational domain so that $\Omega_{l,r}$ becomes the left and the right exterior domain, respectively. When $A_{l,r} = 0$, we obtain the case of compactly supported initial data. The function ϕ can be arbitrary[3] as long as the evolution of the CW background, i.e., initial data of the form

$$u_0(x) = A_0 e^{i\kappa x}, \tag{2}$$

[1] The need for this section was also acknowledged by all the reviewers of the first version of this manuscript. The reader will find that most results in this section have been stated without proof although correspondence with other similar published works is clearly visible.

[2] It must be noted that a well-posedness result for such IVPs with non-vanishing initial data at infinity is not so well established. Further, the usual $L^2(\mathbb{R})$-space does not suffice on account of the infinite energy integral contribution from the CW-background. In fact the correct framework for proving the well-posedness of IVP would be L^p_{loc} or H^s_{loc} spaces. For the nonlinear Schrödinger equation with $\phi = \phi(|u|^2)$, a renormalization procedure can be adopted in order to make the integrals of motion finite [4]. The requirement $u_0(x) \in \mathcal{C}^\infty$ is evidently quite restrictive and it is not known to be a necessary condition for well-posedness of the IVP. In the application of the pseudo-differential approach, the fact that $u(x,t) \in \mathcal{C}^\infty(\mathbb{R}\times\mathbb{R}_+)$, allows us to replace the nonlinear term by an infinitely differentiable potential function. It can be expected that $u_0(x) \in \mathcal{C}^\infty$ is a sufficient condition for this property.

[3] We allow ϕ to be a non-analytic function of the complex variable u, i.e., $\partial_{u*}\phi \neq 0$ where $(*)$ stands for complex conjugation.