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Absorbing boundary conditions for nonlinear acoustics: The Westervelt equation.

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Abstract

We consider the Westervelt equation in an unbounded domain and propose nonlinear absorbing boundary conditions for its efficient and robust numerical simulations. We use the theory of pseudo- and para-differential operators as well as asymptotic expansions to derive local in space and time absorbing boundary conditions of low to high orders in a consistent way. We show that the pseudo- and para-differential theories lead to essentially the same absorbing boundary conditions in terms of computational efficiency and numerical accuracy, whereas the asymptotic expansions result in exactly the same boundary conditions as the ones obtained with the para-differential approach. Moreover, we demonstrate that the use of pseudo- and para-differential operators leads to the same boundary conditions if the nonlinear function to be linearized vanishes at zero. The numerical studies demonstrate both the efficiency and effectiveness of the developed boundary conditions for different regimes of wave propagation in a wide range of excitation frequencies and angles of incidence.

Keywords: Absorbing boundary conditions, Westervelt equation, Nonlinear acoustics, Pseudo-differential operators, Para-differential operators

1 1. Introduction

Many problems in science and engineering are naturally formulated in unbounded domains; typical examples originate from fluid dynamics, solid mechanics, aerodynamics, electrodynamics, acoustics, etc. However, numerical 3 simulations of such problems require a finite computational region. There are basically two approaches which can be 4 used to reformulate problems in infinite domains as problems in finite domains. The first one is to map an unbounded 5 domain to a bounded one, known as the Perfectly Matched Layer technique first introduced by Berenger [11] and later on used for many different partial differential equations. We specifically refer to e.g., [31, 1, 34, 14, 2, 4, 16, 5, 41, 9] in 7 the context of acoustic wave equations. The second approach, followed in this work, is to impose fictitious boundaries 8 to truncate the domain of interest. Such artificial boundaries require special boundary conditions so that the boundary 9 value problem is well-posed and its solution is an accurate approximation to the restriction of the solution in the 10 unbounded domain. In other words, these boundary conditions have to be transparent to or, as they are usually called, 11 absorbing for solutions propagating outwards the artificial boundary. 12 It is commonly recognized that absorbing boundary conditions (ABCs) play a key role in computations on un-13

bounded domains and have a significant impact on the accuracy of numerical methods. Over the past thirty years,

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ABCs have developed into a vigorous research direction including a wide spectrum of methods and approaches. A detailed description of these techniques is out of the scope of this work and therefore we restrict ourselves to referring the reader to the comprehensive review articles [23, 53, 26, 27, 24, 25] and the references therein.

Despite the intensive research activity in the field of transparent boundary conditions, most results have been obtained for linear problems with constant coefficients. Wave equations with variable coefficients have received much less attention, not to mention nonlinear models. There are only few papers devoted to problems with variable coefficients [20], convective [10] and nonlinear [30, 51, 59, 46] terms. Despite the existence of some approaches to the construction of ABCs for nonlinear wave models their application to concrete equations is rather sophisticated and still out of the scope of most research works.

The focus of this work is on the construction of ABCs for high-intensity ultrasound waves governed by the Westervelt equation, which is a basic mathematical model of nonlinear acoustics playing a central role in many medical and industrial applications, such as diagnostic ultrasound [21, 50, 47], thermotherapy of tumors [22, 28, 15], lithotripsy [6], ultrasound cleaning and sonochemistry (e.g. [17, 39]), etc. Linear acoustic models are not applicable to high intensity ultrasound regimes of wave propagation due to appearing nonlinear effects, which require more sophisticated wave equations to be taken into account.

The ABCs proposed in this work are based on two approaches: the theory of pseudo-differential [40, 32, 45] and 30 para-differential [36, 44] calculus. The first approach is applicable to linear wave equations with variable coefficients, 31 therefore we use it for the Westervelt equation linearized in a neighborhood of a reference solution. The second 32 approach we apply directly to the nonlinear Westervelt equation. Notice that both the pseudo- and para-differential 33 theories have already been used in the construction of transparent boundary conditions. For example, the pseudo-34 differential calculus was exploited by Engquist and Majda in [20] to design ABCs for the linear wave equation with 35 variable coefficients. Another application of the pseudo-differential calculus to the construction of ABCs for the acoustic wave equation can be found in [8]. The pseudo-differential approach has also been used to derive ABCs 37 for optical waveguides [7] and the Maxwell equations [3]. Transparent boundary conditions for the semilinear wave 38 equation as well as for the nonlinear Schrödinger equation were obtained in [52] and [51], respectively, with the help 39 of para-differential operators. 40

The novelty of our work lies in the derivation and analysis of high-order ABCs for the Westervelt equation, 41 which have not yet been constructed. We do so for the one- and two-dimensional versions of the Westervelt equation 42 first of all in a domain without corners. It is worth noting that ABCs in general and for the Westervelt equation in 43 particular are used not only when computational domains are infinitely large but also when they are too large for numerical simulations. Specifically, the High Intensity Focused Ultrasound (HIFU) problem considered in this work 45 is a striking example where a finite but still so vast domain of wave propagation occurs that using the entire domain 46 would make computations unfeasible. In the HIFU problem, the use of ABCs is inevitable, since they allow to carry 47 out simulations in domains of order of centimeters (where are the most interesting physical processes take place), 48 otherwise it would require to consider a much larger computational domain to guarantee that the waves leaving the 49 domain were attenuated enough not to influence the physical processes studied. 50

The rest of this paper is organized as follows. In Section 2 we present the problem formulation. In Section 3 we derive absorbing boundary conditions for the Westervelt equation, in one and two space dimensions, based on the pseudo- and para-differential calculus as well as on asymptotic expansions. Section 4 focuses on the Lagrange multiplier based technique to couple the Westervelt equation and ABCs, and on numerical methods to solve the coupled problem. In Section 5 we give numerical results demonstrating the efficiency of the proposed boundary conditions. The paper concludes with a discussion of the main findings.

57 **2. Problem definition**

The Westervelt equation is one of the fundamental equations governing the propagation of acoustic waves in nonlinear regimes [55, 28, 15, 13]. This equation was first derived from Lighthill's equation by Westervelt [55]. In this work, we present a brief derivation of the Westervelt equation from the basic equations of fluid dynamics: the continuity equation, the Navier–Stokes equation, the entropy equation, and the equation of state.

We introduce the pressure p, density ρ , velocity v, specific entropy s, and temperature T, and decompose these

⁶³ quantities into their time-mean and fluctuating components as

$$p = p_0 + p', \tag{1}$$

$$\rho = \rho_0 + \rho', \qquad (2)$$
$$\mathbf{y} = \mathbf{y}_0 + \mathbf{y}'. \qquad (3)$$

$$s = s_0 + s',$$
 (3)

$$T = T_0 + T' \,. \tag{5}$$

⁶⁴ To derive the Westervelt equation, we first consider the equation of continuity

$$\rho_t + \mathbf{v} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{v} = 0. \tag{6}$$

65 Substitution of (1) and (2) into (6) gives

$$(\rho_0 + \rho')_t + \mathbf{v} \cdot \nabla(\rho_0 + \rho') + (\rho_0 + \rho')\nabla \cdot \mathbf{v} = 0.$$
⁽⁷⁾

Assuming the time-mean density ρ_0 to be constant, one can rewrite (7) as

$$\rho_t' + \rho_0 \nabla \cdot \mathbf{v} = -\rho' \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \nabla \rho' \,. \tag{8}$$

⁶⁷ To proceed, we make use of the Navier–Stokes equation

$$\rho\left(\mathbf{v}_{t} + (\mathbf{v} \cdot \nabla)\mathbf{v}\right) + \nabla p = \mu \Delta \mathbf{v} + \left(\zeta + \frac{1}{3}\mu\right)\nabla(\nabla \cdot \mathbf{v}), \qquad (9)$$

with ζ and μ standing for the shear and bulk viscosities, respectively.

69 Applying the vector identities

70

$$\nabla(\nabla \cdot \mathbf{v}) = \Delta \mathbf{v} + \nabla \times \nabla \times \mathbf{v}, \qquad (10a)$$

$$\mathbf{v} \cdot \nabla \mathbf{v} = \frac{1}{2} \nabla (\mathbf{v} \cdot \mathbf{v}) - \mathbf{v} \times \nabla \times \mathbf{v}, \qquad (10b)$$

⁷¹ to the Navier–Stokes equation (9) results in

$$\rho\left(\mathbf{v}_{t} + \frac{1}{2}\nabla(\mathbf{v}\cdot\mathbf{v}) - \mathbf{v}\times\nabla\times\mathbf{v}\right) + \nabla p = \mu\Delta\mathbf{v} + \left(\zeta + \frac{1}{3}\mu\right)(\Delta\mathbf{v} + \nabla\times\nabla\times\mathbf{v}).$$
(11)

Assuming constant p_0 and using (1) and (2), we rewrite (11) in the form

$$(\rho_0 + \rho') \left(\mathbf{v}_t + \frac{1}{2} \nabla (\mathbf{v} \cdot \mathbf{v}) - \mathbf{v} \times \nabla \times \mathbf{v} \right) + \nabla p' = \mu \Delta \mathbf{v} + \left(\zeta + \frac{1}{3} \mu \right) (\Delta \mathbf{v} + \nabla \times \nabla \times \mathbf{v}),$$
(12)

⁷³ which after some rearrangements leads to

$$\rho_0 \mathbf{v}_t + \frac{\rho_0}{2} \nabla (\mathbf{v} \cdot \mathbf{v}) - \rho_0 \mathbf{v} \times \nabla \times \mathbf{v} + \rho' \mathbf{v}_t + \frac{\rho'}{2} \nabla (\mathbf{v} \cdot \mathbf{v}) - \rho' \mathbf{v} \times \nabla \times \mathbf{v} + \nabla p' = \left(\zeta + \frac{4}{3}\mu\right) \Delta \mathbf{v} + \left(\zeta + \frac{1}{3}\mu\right) \nabla \times \nabla \times \mathbf{v} .$$
(13)

Applying (10b) to (13) and taking into account that the acoustic velocity **v** is irrotational in our case ($\nabla \times \mathbf{v} = 0$), equation (13) can be written in the following form

$$\rho_0 \mathbf{v}'_t + \frac{\rho_0}{2} \nabla(\mathbf{v}' \cdot \mathbf{v}') + \rho' \mathbf{v}'_t + \nabla p' = \left(\zeta + \frac{4}{3}\mu\right) \Delta \mathbf{v}',\tag{14}$$

where we also assume zero time-mean velocity \mathbf{v}_0 , which implies the equality $\mathbf{v} = \mathbf{v}'$, and omit the third order fluctuating term $\frac{\rho'}{2} \nabla(\mathbf{v} \cdot \mathbf{v})$.

Another component needed in the derivation is the entropy equation [29]:

$$\rho T \frac{Ds}{Dt} = \kappa \Delta T + \mu (\nabla \cdot \mathbf{v})^2 + \frac{\mu}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial v_k}{\partial x_k} \right)^2, \tag{15}$$

⁷⁹ where *s* is the specific entropy (per unit mass), κ is the thermal conductivity, *T* is the temperature, and δ_{ij} is the ⁸⁰ Kronecker delta.

According to [29], the right hand side of (15) is dominated by the term $\kappa \Delta T'$. We therefore can wirte

$$\rho_0 T_0 \, s'_t = \kappa \Delta T'. \tag{16}$$

⁸² Given the equation of state in the form

$$p = p(\rho, s), \tag{17}$$

we expand it in a Taylor series about an equilibrium state (ρ_0 , s_0) and neglect the third-order terms, namely

$$p - p_0 = \left(P_\rho\right)_{s,0} \left(\rho - \rho_0\right) + \frac{1}{2!} \left(P_{\rho\rho}\right)_{s,0} \left(\rho - \rho_0\right)^2 + \left(P_s\right)_{\rho,0} \left(s - s_0\right) + \dots$$
(18)

Equation (18) can also be expressed as

$$p' = A\left(\frac{\rho'}{\rho_0}\right) + \frac{B}{2}\left(\frac{\rho'}{\rho_0}\right)^2 + (P_s)_{\rho,0} s',$$
(19)

85 with

$$A = \rho_0 \left(P_\rho \right)_{s,0} \equiv \rho_0 c^2, \quad B = \rho_0^2 \left(P_{\rho\rho} \right)_{s,0},$$

where c is the speed of sound, which is assumed to be constant. Thus, equation (19) can be recast into the form

$$p' = c^2 \rho' + \frac{c^2}{\rho_0} \frac{B}{2A} \rho'^2 + (P_s)_{\rho,0} s'.$$
⁽²⁰⁾

In order for the Westervelt equation to be independent of s', we combine the entropy equation (16) and the continuity equation (20). In accordance with [48], we substitute $T' = (T_p)_{s,0} p'$ into (16) that yields

$$\rho_0 T_0 s'_t = \kappa \left(T_p \right)_{s,0} \nabla \cdot \nabla p'.$$
⁽²¹⁾

⁸⁹ From the linear Euler equation

$$\mathbf{v}_t = -\frac{1}{\rho_0} \nabla p',\tag{22}$$

90 we find

$$-\nabla p' = \rho_0 \mathbf{v}_t \tag{23}$$

⁹¹ and substitute it into equation (21):

$$\rho_0 T_0 s'_t = -\rho_0 \kappa \left(T_p \right)_{s,0} (\nabla \cdot \mathbf{v})_t \,. \tag{24}$$

⁹² Then, we integrate equation (24) with respect to time and have

$$\rho_0 T_0 s' = -\rho_0 \kappa \left(T_p\right)_{s,0} \nabla \cdot \mathbf{v},\tag{25}$$

93 Or

$$s' = -\frac{\kappa}{T_0} \left(T_p \right)_{s,0} \nabla \cdot \mathbf{v} \,. \tag{26}$$

⁹⁴ Substitution of (26) into (20) yields

$$p' = c^2 \rho' + \frac{c^2}{\rho_0} \frac{B}{2A} \rho'^2 - \frac{\kappa}{T_0} (P_s)_{\rho,0} (T_p)_{s,0} \nabla \cdot \mathbf{v}.$$
 (27)

In order to compute the coefficient $\frac{1}{T_0} (P_s)_{\rho,0} (T_p)_{s,0}$ in (27), we use the equation of state for a perfect gas [48], which gives

$$p' = c^2 \rho' + \frac{c^2}{\rho_0} \frac{B}{2A} {\rho'}^2 - \kappa \left(\frac{1}{c_v} - \frac{1}{c_p}\right) \nabla \cdot \mathbf{v}.$$
(28)

⁹⁷ Using the linear equation of continuity

$$\nabla \cdot \mathbf{v} \approx -\frac{1}{\rho_0} \rho_t' \,. \tag{29}$$

98 in (28) results in

$$p' = c^2 \rho' + \frac{c^2}{\rho_0} \frac{B}{2A} \rho'^2 + \frac{\kappa}{\rho_0} \left(\frac{1}{c_v} - \frac{1}{c_p}\right) \rho'_t.$$
(30)

⁹⁹ On the other hand, from the linear equation of state

$$\rho' = p'c^{-2},\tag{31}$$

¹⁰⁰ it follows that (30) can be written as

$$p' = c^2 \rho' + \frac{1}{\rho_0 c^2} \frac{B}{2A} p'^2 + \frac{\kappa}{\rho_0 c^2} \left(\frac{1}{c_v} - \frac{1}{c_p}\right) p'_t.$$
(32)

Multiplication of equation (32) by c^{-2} and expressing it in terms of ρ' gives

$$\rho' = \frac{p'}{c^2} - \frac{1}{\rho_0 c^4} \frac{B}{2A} p'^2 - \frac{\kappa}{\rho_0 c^4} \left(\frac{1}{c_v} - \frac{1}{c_p}\right) p'_t.$$
(33)

The next step is to combine the equation of continuity (8), the momentum equation (14) and the equation of state (33) into one equation. For doing so, we first use (29) and (31) to recast (8) in the form

$$\rho_t' + \rho_0 \nabla \cdot \mathbf{v} = \frac{p'}{\rho_0 c^4} p_t' - \frac{1}{c^2} \mathbf{v} \cdot \nabla p'.$$
(34)

¹⁰⁴ We then differentiate equation (33) with respect to time

$$\rho_t' = \frac{1}{c^2} p_t' - \frac{1}{\rho_0 c^4} \frac{B}{2A} \left(p'^2 \right)_t - \frac{\kappa}{\rho_0 c^4} \left(\frac{1}{c_v} - \frac{1}{c_p} \right) p_{tt}'$$
(35)

and use (34) to have

$$\frac{1}{c^2}p'_t - \frac{1}{\rho_0 c^4} \frac{B}{2A} \left(p'^2\right)_t - \frac{\kappa}{\rho_0 c^4} \left(\frac{1}{c_v} - \frac{1}{c_p}\right) p'_{tt} + \rho_0 \nabla \cdot \mathbf{v} = \frac{1}{2\rho_0 c^4} \left(p'^2\right)_t - \frac{1}{c^2} \mathbf{v} \cdot \nabla p' \,. \tag{36}$$

¹⁰⁶ Using equations (22), (31) to express the term $\rho' \mathbf{v}'_t$ and equations (29), (31) to express the term $\left(\zeta + \frac{4}{3}\mu\right)\Delta\mathbf{v}'$, one ¹⁰⁷ can reformulate the Navier–Stokes equation (14) as

$$\rho_0 \mathbf{v}_t + \nabla p' = \frac{1}{2\rho_0 c^2} \nabla p'^2 - \frac{\rho_0}{2} \nabla (\mathbf{v} \cdot \mathbf{v}) - \frac{1}{\rho_0 c^2} \left(\zeta + \frac{4}{3} \mu \right) \nabla p'_t.$$
(37)

¹⁰⁸ Application of the divergence operator to (37) gives

$$\rho_0 \left(\nabla \cdot \mathbf{v}_t \right) + \Delta p' = \frac{1}{2\rho_0 c^2} \Delta p'^2 - \frac{\rho_0}{2} \Delta (\mathbf{v} \cdot \mathbf{v}) - \frac{1}{\rho_0 c^2} \left(\zeta + \frac{4}{3} \mu \right) \Delta p'_t \,. \tag{38}$$

¹⁰⁹ Differentiation of (36) with respect to time and subtraction the resulting equation from (38) leads to

$$\Delta p' - \frac{1}{c^2} p'_{tt} = \frac{1}{2\rho_0 c^2} \Delta p'^2 - \frac{\rho_0}{2} \Delta (\mathbf{v} \cdot \mathbf{v}) - \frac{1}{\rho_0 c^2} \left(\zeta + \frac{4}{3}\mu\right) \Delta p'_t - \frac{1}{\rho_0 c^4} \frac{B}{2A} \left(p'^2\right)_{tt} - \frac{\kappa}{\rho_0 c^4} \left(\frac{1}{c_v} - \frac{1}{c_p}\right) p'_{ttt} - \frac{1}{2\rho_0 c^4} \left(p'^2\right)_{tt} - \frac{\rho_0}{2c^2} \left(\mathbf{v} \cdot \mathbf{v}\right)_{tt} .$$
(39)

After rearrangement of the right hand side in (39) and using the replacements

$$\Delta(\mathbf{v}\cdot\mathbf{v}) = c^{-2} (\mathbf{v}\cdot\mathbf{v})_{tt}, \quad \Delta p' = c^{-2} p'_{tt},$$

in the higher order terms we arrive at Kuznetsov's equation, which governs the propagation of nonlinear waves in a thermoviscous medium,

$$\frac{1}{c^2}p'_{tt} - \Delta p' - \frac{\delta}{c^4}p'_{ttt} = \left(\frac{1}{\rho_0 c^4} \frac{B}{2A} p'^2 + \frac{\rho_0}{c^2} \mathbf{v} \cdot \mathbf{v}\right)_{tt},$$
(40)

where the diffusivity of sound $\delta > 0$ is given, as presented in [42], by

$$\delta = \frac{1}{\rho_0} \left(\zeta + \frac{4}{3} \mu \right) + \frac{\kappa}{\rho_0} \left(\frac{1}{c_v} - \frac{1}{c_p} \right),$$

Assuming that local nonlinear effects can be neglected, (i.e., making the replacement $\mathbf{v} \cdot \mathbf{v} = \left(\frac{1}{\rho_0 c} p'\right)^2$ on the right hand side) we arrive at the Westervelt equation

$$\frac{1}{c^2}p'_{tt} - \Delta p' - \frac{\delta}{c^4}p'_{ttt} = \frac{\beta_a}{\rho_0 c^2} (p'^2)_{tt}, \qquad (41)$$

and inserting the linear wave equation relation for the damping term (i.e. $c^{-2}p'_{ttt} = \Delta p'_t$), the Westervelt equation (41) can be written as

$$\frac{1}{c^2}u_{tt} - \Delta u - \frac{\delta}{c^2}\Delta u_t = \frac{\beta_a}{\rho_0 c^2} (u^2)_{tt}, \quad \text{in} \ (0,T) \times \Omega \,, \quad u := p', \tag{42}$$

and $\Omega \subseteq \mathbb{R}^d$, $d \in \{1, 2, 3\}$, $u = u(\cdot, t)$ is the acoustic pressure, $\beta_a = 1 + B/(2A)$ with B/(2A) > 0 standing for the parameter of nonlinearity of the fluid, and *T* is the final time at which the problem is to be solved. All the parameters are assumed to be constant.

The Westervelt equation (41) is widely used to simulate high-intensity focused ultrasound fields generated by medical ultrasound transducers. This equation is valid when the cumulative nonlinear effects dominate the local nonlinear effects. Unlike the Khokhlov-Zabolotskaya-Kuznetsov equation, which is valid for directional sound beams and can be applied for transducers with relatively small aperture angles, the Westervelt equation allows using largeaperture-angle transducers.

In some cases the dimensionless form of the Westervelt equation [54] is more preferable than its dimensional analogue. However, for the purpose of this paper, we use the dimensional version of the equation. It is also worth noting that the classical Westervelt equation derived in [55] is an equation which is obtained from (41) by setting $\delta = 0$. Despite this fact, equation (41) is also referred to as the Westervelt equation.

We recast the Westervelt equation (42) in a form more convenient for further treatment

$$c^{-2}u_{tt} - \Delta u - \beta \Delta u_t = \gamma(u^2)_{tt} \quad \text{in } (0, T) \times \Omega$$
(43)

with $\beta = \delta/c^2$, $\gamma = \beta_a/(\rho_0 c^4)$, and complement (43) with the initial conditions

$$u(\cdot, t = 0) = u_0, \quad u_t(\cdot, t = 0) = u_1 \quad \text{in } \Omega,$$
(44)

and with the inhomogeneous Neumann and absorbing boundary conditions

$$u_n\Big|_{(0,T)\times\Gamma_{\rm N}} = g(t), \quad \mathcal{A}u\Big|_{(0,T)\times\Gamma_{\rm A}} = 0, \tag{45}$$

where Γ_N is a boundary part on which excitation of sound takes place, and Γ_A is an artificial boundary part on which absorbing boundary conditions are prescribed; $\partial \Omega = \Gamma_N \cup \Gamma_A$, *n* is the normal derivative to the boundary Γ_N and the operator \mathcal{A} is an annihilating operator for outgoing waves, which we specify in due course.

3. Absorbing boundary conditions for the Westervelt equation

In our derivation, without loss of generality we consider two domains $\Omega = (-\infty, 0]$ in 1-d and $\Omega = (-\infty, 0] \times \mathbb{R}$ in 2-d, where *x* plays the role of the outward unit normal and (in 2-d) *y* is the tangential direction.

¹³⁹ 3.1. Absorbing boundary conditions in 1-d via linearization and pseudo-differential calculus

As it was already mentioned, the direct reformulation of the Westervelt equation (43) in terms of pseudo-differential operators is not possible because of the nonlinear term on the right hand side. Therefore, we linearized (43) around a reference solution $u^{(0)}$

$$(c^{-2} - 2\gamma u^{(0)})u_{tt} - \Delta u - \beta \Delta u_t = 2\gamma u_t^{(0)} u_t \quad \text{in} \ (0, T) \times \Omega \,.$$
(46)

After the derivation of the ABCs from this inhomogeneous linear wave equation with variable coefficients, we reinsert $u^{(0)} = u$ to arrive at the ABCs for the Westervelt equation. The reason for using (46) (as was also done for the well-posedness proof in [37]) and not the standard linearization according to the first order Taylor expansion, which would be

$$c^{-2}u_{tt} - \Delta u - \beta \Delta u_t = 2\gamma \Big(2u_t^{(0)} u_t + u u_{tt}^{(0)} + u^{(0)} u_{tt} - (u_t^{(0)})^2 - u^{(0)} u_{tt}^{(0)} \Big) \quad \text{in } (0, T) \times \Omega \,, \tag{47}$$

is that the offset terms $-2(u_t^{(0)})^2 - 2u^{(0)}u_{tt}^{(0)} = -\gamma(u^{(0)})_{tt}^2$ would destroy the commutativity of symbols of pseudodifferential operators below.

¹⁴⁹ For simplicity of exposition we first of all consider the one-dimensional version of the Westervelt equation (43)

$$c^{-2}u_{tt} - u_{xx} - \beta u_{txx} = \gamma(u^2)_{tt} \,. \tag{48}$$

¹⁵⁰ Thus, in 1-d the operator form of linearization (46) reads as

$$\mathfrak{D}_1 u = 0, \quad \text{with } \mathfrak{D}_1 = v^2 \partial_t^2 - \partial_x^2 - \beta \partial_{txx} - 2\gamma u_t^{(0)} \partial_t \,,$$
(49)

151 where we set $v^2 = v^2(u^{(0)})$ with

$$v^2(v) = c^{-2} - 2\gamma v, (50)$$

and point out that our analysis of the Westervelt equation, cf. [38], is based on estimates that actually make sure positivity of $c^{-2} - 2\gamma u$, so that $v^2 > 0$ is a natural assumption. In order to derive transparent boundary conditions for the linearized Westervelt equation (48) we make use of the theory of pseudo-differential calculus. For the purpose of this formal derivation, v is assumed to be a C^{∞} function both in time and space. Otherwise further discussion based on pseudo-differential operators makes no sense due to the impossibility to associate a differential operator with a symbol having a limited regularity. Since we do not prove this smoothness, our derivations are only formal.

¹⁵⁸ Our derivation of ABCs is based on the Nirenberg factorization of (49) written in terms of pseudo-differential ¹⁵⁹ operators. Thus, to construct approximate boundary conditions we factorize the operator \mathfrak{D}_1 as

$$\mathfrak{D}_1 = -(\partial_x - A)(\partial_x - B) + R, \tag{51}$$

where $A = A(x, t, D_t)$ and $B = B(x, t, D_t)$ are pseudo-differential operators with symbols $a(x, t, \tau)$ and $b(x, t, \tau)$ from the space

$$S^{1} = S^{1}(\mathbb{R}^{2}) = \left\{ f(t,\tau) \in C^{\infty}(\mathbb{R}^{2}) : \left| \frac{\partial^{\xi}}{\partial t^{\xi}} \frac{\partial^{\sigma}}{\partial \tau^{\sigma}} f(t,\tau) \right| \le C_{\xi,\sigma} (1+|\tau|)^{1-|\sigma|}, \ \forall \xi, \sigma \in \mathbb{N}_{0} \right\}.$$

The differential operator D_t is defined as $-i\partial_t$ with the imaginary unit *i*, and *R* is a smoothing pseudo-differential operator with the Schwartz kernel $k(x, y) \in C^{\infty}$ satisfying [33]:

$$(1+|x-y|)^N \left| \frac{\partial^{\xi}}{\partial x^{\xi}} \frac{\partial^{\sigma}}{\partial y^{\sigma}} k(x,y) \right| \le C_{\xi,\sigma,N}, \quad \forall \xi, \sigma, N \in \mathbb{N}_0.$$

¹⁶⁴ Developing factorization (51), we get

$$\mathfrak{D}_1 = -\partial_x^2 + (A+B)\partial_x + B_x - AB + R.$$
(52)

¹⁶⁵ At the symbolic level, factorization (52) reduces to

$$\nu^{2}(i\tau)^{2} - \beta(i\tau)\partial_{x}^{2} - 2\gamma u_{t}^{(0)}(i\tau) = (a+b)\partial_{x} + b_{x} - ab + R$$
(53)

- with the correspondence $i\tau \leftrightarrow \partial_t$ between the frequency and the (physical) time domains. By a slight abuse of notation,
- ¹⁶⁷ for a function f, we denote the symbol of the zero order differential operators $u \mapsto fu$ (multiplication operator) again
- 168 by f.
- The next step is to define symbols a and b in (53). For doing so, it is worth to remark that formally these symbols
- admit the following asymptotic expansions

$$a(x,t,\tau) \sim \sum_{j \ge 0} a_{1-j}(x,t,\tau), \quad |\tau| \to \infty,$$
(54a)

171 and

$$b(x,t,\tau) \sim \sum_{j \ge 0} b_{1-j}(x,t,\tau), \quad |\tau| \to \infty,$$
 (54b)

where $a_{1-j}(x, t, \tau)$ and $b_{1-j}(x, t, \tau)$ are homogeneous functions of degree 1 - j in τ . To asymptotically expand the symbol c := ab, we make use of the following theorem [58].

Theorem 3.1. The product of two pseudo-differential operators $A(\mathbf{x}, D) \in \Psi^{m_1}$ and $B(\mathbf{x}, D) \in \Psi^{m_2}$ with symbols a($\mathbf{x}, \boldsymbol{\xi}$) $\in S^{m_1}$ and b($\mathbf{x}, \boldsymbol{\xi}$) $\in S^{m_2}$ respectively, is a composition operator $C(\mathbf{x}, D) = A(\mathbf{x}, D)B(\mathbf{x}, D) \in \Psi^{m_1+m_2}$ with a symbol $c(\mathbf{x}, \boldsymbol{\xi}) \in S^{m_1+m_2}$ having the asymptotic expansion given by

$$c(\mathbf{x},\boldsymbol{\xi}) \sim \sum_{|\alpha| \le N} \frac{1}{\alpha!} D_{\boldsymbol{\xi}}^{\alpha} a(\mathbf{x},\boldsymbol{\xi}) \partial_{x}^{\alpha} b(\mathbf{x},\boldsymbol{\xi})$$
(55)

177 for every nonnegative integer N and with the standard multi-index notation $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_k), |\alpha| = \alpha_1 + \alpha_2 + \dots + \alpha_k$

x = $(x_1, x_2, ..., x_k)$, $\boldsymbol{\xi} = (\xi_1, \xi_2, ..., \xi_k)$, $D^{\alpha} = D^{\alpha_1} D^{\alpha_2} ... D^{\alpha_k}$ and $\partial^{\alpha} = \partial^{\alpha_1} \partial^{\alpha_2} ... \partial^{\alpha_k}$. Thus, the symbol c := ab of the product of the pseudo-differential operators $A(x, t, D_t)$ and $B(x, t, D_t)$ is asymptotic to

$$c(x,t,\tau) \sim \sum_{k,l,n\geq 0} \frac{(-i)^n}{n!} \partial_{\tau}^n a_{1-k}(x,t,\tau) \partial_t^n b_{1-l}(x,t,\tau) \,.$$
(56)

Substitution of (54) and (56) in (53) and casting-out *R* lead to

$$v^{2}(i\tau)^{2} - \beta(i\tau)\partial_{x}^{2} - 2\gamma u_{t}^{(0)}(i\tau) = \sum_{j\geq0} (a_{1-j} + b_{1-j})\partial_{x} + \sum_{j\geq0} \partial_{x}b_{1-j} - \sum_{j\geq0, \, k+l+n=j} \underbrace{\left(\frac{(-i)^{n}}{n!}\partial_{\tau}^{n}a_{1-k}\partial_{t}^{n}b_{1-l}\right)}_{O(\tau^{2-j})}, \quad k, l, n \geq 0.$$
(57)

By equating the symbols with the same degree of homogeneity on both sides of equation (57) we can find the coefficients a_{1-j} and b_{1-j} for $j \ge 0$. Typically, the more coefficients are taken the more accurate ABCs are. However, taking more coefficients also makes the ABCs more complicated and involved to implement, since they contain higher order derivatives. Therefore, we only show how to find the coefficients $\{a_j, b_j\}_{j=\{1,0,-1\}}$ and note that other coefficients can be calculated analogously. In order to define the first pair of coefficients a_1 and b_1 , we equate the symbols with the degree of homogeneity $O(\tau^2)$. This gives the system of equations

$$\begin{cases} a_1 + b_1 = 0, \\ v^2(i\tau)^2 = -a_1b_1. \end{cases}$$
(58)

¹⁸⁷ To make the terms of order $O(\tau^2)$ vanish we took the following solution to (58)

$$b_1 = -a_1 = \nu(i\tau). \tag{59}$$

Remark 3.1. The choice of the sign in front of $v(i\tau)$ is not arbitrary, since it defines the propagation direction of the wave. In order to find the next pair of coefficients a_0 , b_0 we equate the symbols with degree of homogeneity $O(\tau^1)$ that gives the following system of equations

$$\begin{cases} a_0 + b_0 = 0, \\ \beta(i\tau)\partial_x^2 + 2\gamma u_t^{(0)}(i\tau) = a_1 b_0 + a_0 b_1 - i a_{1\tau} b_{1t} - b_{1x}, \end{cases}$$
(60)

in terms of unknowns a_0, b_0 .

Substitution of $b_1 = -a_1$ in (60) yields

$$b_0 = -a_0 = -\frac{1}{2a_1} \left(ia_{1\tau} a_{1t} + a_{1x} - \beta(i\tau) \partial_x^2 - 2\gamma u_t^{(0)}(i\tau) \right)$$
(61)

¹⁹⁴ or, in terms of $a_1 = -\nu(i\tau)$, we have

$$b_0 = -a_0 = -\frac{1}{2\nu} \left(\mathcal{A}_0[\nu] + \beta \partial_x^2 + 2\gamma u_t^{(0)} \right)$$
(62)

¹⁹⁵ with the operator $\mathcal{A}_0 := \partial_x + \nu \partial_t$.

Remark 3.2. Note that here we exchanged the order of b_0 and a_1 . However, with a_1 , b_0 , a_0 as above this is obviously 196 not correct as long as $\beta \neq 0$ since, for example, in a_0b_1 the second order space derivative from a_0 acts on the function 197 v from b_1 . These difficulties are caused by the strong damping term $\beta\Delta u$ in deriving ABCs, and have a quite natural 198 explanation: The strong damping term destroys the wave like character of the equation since it implies decay of the 199 energy and a rather parabolic than hyperbolic behaviour of the equation, cf. [37]. Moreover, note that the β term 200 would lead to a second order normal derivative term in the first order and even to a fourth order normal derivative 201 term in the second order absorbing boundary conditions. Vanishing β enables us to recover commutativity of the 202 operators a_1 and b_0 as required to justify the derivations above. In the following we omit the term with β in (62) i.e. 203 consider 204

$$b_0 = -a_0 = -\frac{1}{2\nu} \left(\mathcal{A}_0[\nu] + 2\gamma u_t^{(0)} \right)$$
(63)

instead, and also set $\beta = 0$ in the further derivation of absorbing boundary conditions.

In order to obtain more accurate boundary conditions we equate the symbols with degree of homogeneity $O(\tau^0)$, which leads to the following system of equations

$$\begin{cases} a_{-1} + b_{-1} = 0, \\ -a_{1}b_{-1} - a_{0}b_{0} - a_{-1}b_{1} + i(a_{1\tau}b_{0t} + a_{0\tau}b_{1t}) - \frac{i^{2}}{2}a_{1\tau\tau}b_{1tt} + b_{0x} = 0. \end{cases}$$
(64)

The solution to (64) is given by

$$b_{-1} = -a_{-1} = -\frac{1}{2a_1} \left(-a_0^2 + i(a_{1\tau}a_{0t} + a_{0\tau}a_{1t}) + \frac{1}{2}a_{1\tau\tau}a_{1tt} + a_{0x} \right).$$
(65)

²⁰⁹ Taking into account (59) and (62) we deduce that

$$b_{-1} = -a_{-1} = \frac{1}{2\nu(i\tau)} \left(\mathcal{A}_0 \left[\frac{1}{2\nu} \left(\mathcal{A}_0[\nu] + 2\gamma u_t^{(0)} \right) \right] - \left(\frac{1}{2\nu} \left(\mathcal{A}_0[\nu] + 2\gamma u_t^{(0)} \right) \right)^2 \right) =: \frac{\gamma \mu}{2\nu(i\tau)} .$$
(66)

Again we have exchanged the order of the operators to have $a_1b_{-1} + a_{-1}b_1 = a_1b_{-1} - a_{-1}a_1 = a_1(b_{-1} - a_{-1})$. Having set $\beta = 0$ helps here as well, since this renders $a_{-1}(x, t, D_t)D_t$ a plain multiplication operator. Note that with the Taylor linearization (47) an offset term $\gamma(u^{(0)^2})_{tt}$ would have appeared here, which would have prevented the equality $a_{-1}a_1 = a_1a_{-1}$. (Here, we write f for the symbol of the zero order differential operator $u \mapsto f$ (constant mapping), which has to be strictly distinguished from the multiplication operator $u \mapsto fu$.) This problem is avoided by using the fixed point type linearization (46).

According to [43], the operator 216

$$\partial_x - a(x, t, D_t) = 0 \tag{67}$$

annihilates outgoing waves at $\{x = 0\} \times (0, T)$ and thus can be used to construct ABCs of different orders of accuracy. 217 Substitution of the asymptotic expansion (54a) with the first k leading terms into (67) results in the following boundary 218 condition 219

$$\left(\partial_{x} - \sum_{j=0}^{k} a_{1-j}(x, t, D_{t})\right) u \bigg|_{x=0} = 0.$$
(68)

An ABC of order *k* can be obtained from (68) by keeping the first *k* terms. 220

Thus, in order to construct a zero order ABC we set k = 0 and substitute the coefficient a_1 in (68), which gives 221

$$\mathcal{A}_0[u]\Big|_{x=0} = (u_x + vu_t)\Big|_{x=0} = 0.$$
(69)

Parallel to the construction of the zero order ABC (69), we set k = 1 and substitute a_1, a_0 in (68) to obtain the first 222 order boundary condition: 223

$$\mathcal{A}_{1}u\Big|_{x=0} = (\mathcal{A}_{0} - \mathcal{B}_{1})u\Big|_{x=0} = \left(u_{x} + \nu u_{t} - \frac{1}{2\nu}\left((\nu_{x} + \nu \nu_{t})u + 2\gamma u_{t}^{(0)}u\right)\right)\Big|_{x=0} = 0$$
(70)

with $\mathcal{B}_1 := \frac{1}{2\nu} \left(\mathcal{A}_0[\nu] + 2\gamma u_t^{(0)} \right)$. For k = 2 we obtained the second order ABC 224

225

$$\mathcal{A}_{2}u\Big|_{x=0} = \left(\mathcal{A}_{1}u_{t} - \mathcal{B}_{2}u\right)\Big|_{x=0} = \left(u_{xt} + \nu u_{tt} - \frac{1}{2\nu}\left((\nu_{x} + \nu\nu_{t})u_{t} + 2\gamma u_{t}^{(0)}u_{t} - \mu u\right)\right)\Big|_{x=0} = 0,$$
(71)

where we multiplied with $(i\tau)$ before converting from symbols to operators, and where $\mathcal{B}_2 := \frac{\gamma \mu(u^{(0)})}{2\nu(u^{(0)})}$ with 226

$$\mu(\nu) = \frac{1}{\gamma} \mathcal{A}_0 \left[\frac{1}{2\nu(\nu)} \left(\mathcal{A}_0[\nu(\nu)] + 2\gamma\nu_t \right) \right] - \left(\frac{1}{2\nu(\nu)} \left(\mathcal{A}_0[\nu(\nu)] + 2\gamma\nu_t \right) \right)^2 \\ = \mathcal{A}_0 \left[\frac{1}{2\sqrt{c^{-2} - 2\gamma\nu}} \left(-\frac{\nu_x}{\sqrt{c^{-2} - 2\gamma\nu}} + \nu_t \right) \right] - \gamma \left(\frac{1}{2\sqrt{c^{-2} - 2\gamma\nu}} \left(-\frac{\nu_x}{\sqrt{c^{-2} - 2\gamma\nu}} + \nu_t \right) \right)^2.$$
(72)

Inserting *u* itself for the a priori solution $u^{(0)}$, we arrive at zero 227

$$\left(u_{x} + \sqrt{c^{-2} - 2\gamma u} u_{t}\right)\Big|_{x=0} = 0,$$
(73)

first 228

$$\left(u_{x} + \sqrt{c^{-2} - 2\gamma u} u_{t} - \frac{\gamma}{2\sqrt{c^{-2} - 2\gamma u}} \left(u_{t}u - \frac{1}{\sqrt{c^{-2} - 2\gamma u}} u_{x}u\right)\right)\Big|_{x=0} = 0,$$
(74)

and second order 229

$$\left(u_{xt} + \sqrt{c^{-2} - 2\gamma u} u_{tt} - \frac{\gamma}{2\sqrt{c^{-2} - 2\gamma u}} \left((u_t)^2 - \frac{1}{\sqrt{c^{-2} - 2\gamma u}} u_x u_t - \mu(u) u \right) \right) \Big|_{x=0} = 0$$
(75)

nonlinear ABCs for the Westervelt equation (48). Note that slightly different boundary conditions result from the 230 231 derivation via the para-differential approach presented in Section 3.2.

10

232 3.2. Absorbing boundary conditions in 1-d via para-differential calculus

In this part, we focus on the construction of absorbing boundary conditions for the Westervelt equation (43) with no 233 234 preliminary linearization in contrast to the approach used in Section 3.1. The disadvantage of the pseudo-differential approach for designing ABCs is in its inability to treat nonlinear equations. This obstacle can be overcome by using the 235 para-differential calculus originated from the paper of Bony [36] with an improvement done by Meyer [44]. Although 236 the para-differential calculus and especially Bony's para-linearization technique embrace wide opportunities to build 237 ABCs for nonlinear equations, their use is still very restricted in current research works. The first application of para-238 differential operators to the development of ABCs has been done for the Burgers equation in [18]. Some relatively 239 recent results can be found in few works (e.g. [52, 51]). 240

Before the derivation of ABCs we briefly recall some general facts about para-differential operators and Bony's para-linearization. Let us consider a nonlinear differential equation of order *N* defined as follows

$$F[u](x) = \Phi(x, u(x), \dots, \partial^{\alpha} u(x), \dots)_{0 < |\alpha| < N} = 0$$
(76)

with $\Phi \in C^{\infty}$ and $x \in \mathbb{R}^d$. In accordance to [36], the para-linearization of (76) with $\Phi(x, \cdot)$ vanishing at 0 is given by

$$F[u] = \sum_{0 \le |\alpha| \le N} T_{F'(u)} \partial^{\alpha} u + R(u), \qquad (77)$$

where $T_{F'(u)}$ is a para-differential operator having as symbol the linearization $F'(u) = \frac{\partial \Phi}{\partial \lambda_a}(\cdot, u, \dots, \partial^{\alpha} u, \dots)_{0 \le |\alpha| \le N}$ of Fat u, and R(u) is a smooth error. More precisely, for all $u \in H^s(\mathbb{R}^d)$ with s > d/2 equation (77) implies $R(u) \in H^{2s-d/2}$ (see [44]). Equation (77) is often referred to as the para-linearization formula of Bony, and the para-differential operator T_a with a symbol $a(x) \in C^{\infty}$, $x \in \mathbb{R}^d$ is defined as

$$\mathcal{F}(T_a u)(\zeta) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \chi(\zeta - \eta, \eta) \mathcal{F}a(\zeta - \eta) \mathcal{F}u(\eta) \, d\eta \,, \tag{78}$$

where \mathcal{F} is the Fourier transform, and $\chi \in C^{\infty}(\mathbb{R}^d \times \{\mathbb{R}^d \setminus \{0\}\})$ is a function of homogeneity degree zero satisfying

$$\begin{cases} \chi(\zeta,\eta) = 1 & \text{if } |\zeta| \le \varepsilon_1 |\eta|, \\ \chi(\zeta,\eta) = 0 & \text{if } |\zeta| \ge \varepsilon_2 |\eta|, \end{cases}$$
(79)

with $0 < \varepsilon_1 < \varepsilon_2$.

Before the derivation of ABCs for the Westervelt equation (48), we develop the nonlinear term on its right hand side $\gamma(u^2)_{tt} = 2\gamma((u_t)^2 + uu_{tt})$ and recast (48) in the form

$$v^{2}(u)u_{tt} - u_{xx} - \beta u_{txx} = 2\gamma(u_{t})^{2}$$
(80)

with $v^2(u) = c^{-2} - 2\gamma u$.

Based on (77) and taking into account that the product of two functions f and g can be written in term of paradifferential operators [36] as

$$fg = T_f g + T_g f + R, ag{81}$$

where T_f and T_g are para-differential operators with symbols f and g, we obtain the para-linearized Westervelt equation in the operator form

$$\mathfrak{D}_2 u = 0, \quad \mathfrak{D}_2 = c^{-2} \partial_t^2 - 2\gamma (T_{u_{tt}} + T_u \partial_t^2) - \partial_x^2 - \beta \partial_{txx} - 2\gamma T_{2u_t} \partial_t \tag{82}$$

²⁵⁷ instead of the Westervelt equation (80).

Acting similar to the previous derivation, we apply Nirenberg's factorization, analogous to (51), and rewrite (82) in the form

$$\mathfrak{D}_2 = -(\partial_x - A)(\partial_x - B) + R, \qquad (83)$$

where A and B are para-differential operators with symbols a and b, respectively.

A similar argument as for the linearized Westervelt equation yields

$$v^{2}(u)(i\tau)^{2} - 2\gamma u_{tt} - \beta(i\tau)\partial_{x}^{2} - 4\gamma u_{t}(i\tau) = (a+b)\partial_{x} + \partial_{x}b - ab + R.$$
(84)

²⁶² Note that this equation differs from (53) and also leads to different ABCs. Again, we skip the β terms for the same ²⁶³ reason as in Section 3.1.

Substitution of asymptotic expansions of symbols (54) and (55) in (84) results in equation (57) from which, by

equating the symbols of the same degree of homogeneity $O(\tau^2)$ on both sides, we obtain the same coefficients

$$b_1 = -a_1 = v(i\tau).$$
 (85)

However, the equation for the $O(\tau^1)$ terms is different compared to (60), namely

$$\begin{cases} a_0 + b_0 = 0, \\ \beta(i\tau)\partial_x^2 + 4\gamma u_t^{(0)}(i\tau) = a_1b_0 + a_0b_1 - ia_{1\tau}b_{1t} - b_{1x}, \end{cases}$$
(86)

which upon setting $\beta = 0$ yields (as opposed to (63))

$$b_0 = -a_0 = -\frac{1}{2\nu} \left(\mathcal{A}_0[\nu] + 4\gamma u_t \right)$$
(87)

- with the operator $\mathcal{A}_0 := \partial_x + v \partial_t$.
- Finally, in contrast to (64), we have the following equation for the $O(\tau^0)$ terms

$$\begin{cases} a_{-1} + b_{-1} = 0, \\ -a_{1}b_{-1} - a_{0}b_{0} - a_{-1}b_{1} + i(a_{1\tau}b_{0t} + a_{0\tau}b_{1t}) - \frac{i^{2}}{2}a_{1\tau\tau}b_{1tt} + b_{0x} = -2\gamma u_{tt}, \end{cases}$$
(88)

270 so that we get

$$b_{-1} = -a_{-1} = \frac{1}{2\nu(i\tau)} \left(\mathcal{A}_0 \left[\frac{1}{2\nu} \left(\mathcal{A}_0[\nu] + 4\gamma u_t \right) \right] - \left(\frac{1}{2\nu} \left(\mathcal{A}_0[\nu] + 4\gamma u_t \right) \right)^2 - 2\gamma u_{tt} \right) =: \frac{\tilde{\mu}}{2\nu(i\tau)} \,. \tag{89}$$

Parallel to the ABCs for the linearized Westervelt equation from Section 3.1, we obtained the zero order ABC

$$\mathcal{H}'_{0}u\big|_{x=0} = (\partial_{x} + \nu(u)\partial_{t}) \, u\big|_{x=0} = 0\,, \tag{90}$$

272 the first order one

$$\mathcal{R}_{1}' u \Big|_{x=0} = \left(\mathcal{R}_{0}' - \mathcal{B}_{1}' \right) u \Big|_{x=0} = \left(\partial_{x} + \nu(u) \partial_{t} - \frac{1}{2\nu(u)} \left(\mathcal{R}_{0}' [\nu(u)] + 4\gamma u_{t} \right) \right) u \Big|_{x=0} = 0,$$
(91)

with $\mathcal{B}'_1 := \frac{1}{2\nu(u)}(\mathcal{A}'_0[\nu] + 4\gamma u_t)$, and the second order boundary condition

$$\mathcal{R}_{2}'u\Big|_{x=0} = \left(\mathcal{R}_{1}'u_{t} - \mathcal{B}_{2}'u\right)\Big|_{x=0} = \left(u_{xt} + vu_{tt} - \frac{1}{2\nu}\left((v_{x} + vv_{t})u_{t} + 4\gamma(u_{t})^{2} - \tilde{\mu}u\right)\right)\Big|_{x=0} = 0,$$
(92)

where $\mathcal{B}'_2 := \tilde{\mu}(u)$, which contains multiplication with u_{tt} , as opposed to (71). As in the pseudo-differential case, we do not consider higher order boundary conditions, although their derivation follows the same lines.

276 3.3. Absorbing boundary conditions in 1-d via asymptotic expansions

An alternative approach to the derivation of ABCs for the Westervelt equation (48) can be based on the asymptotic expansion of the solution u(x, t) in an ε -neighborhood of $u^{(0)}(x, t)$ in terms of ε , namely

$$u = u^{(0)} + \varepsilon u^{(1)} + \varepsilon^2 u^{(2)} + \dots$$
(93)

For the purposes pursued in this work it is enough to consider the terms of order ε in (93). Plugging (93), up to the terms $O(\varepsilon^1)$, into (48) gives

$$c^{-2}(u^{(0)} + \varepsilon u^{(1)})_{tt} - (u^{(0)} + \varepsilon u^{(1)})_{xx} - \beta (u^{(0)} + \varepsilon u^{(1)})_{txx} = \gamma (u^{(0)^2} + 2\varepsilon u^{(0)}u^{(1)} + \varepsilon^2 u^{(1)^2})_{tt}.$$
(94)

²⁸¹ The standard asymptotic argument implies equating the terms of the same degree in ε . In particular, for $O(\varepsilon^0)$ we ²⁸² have

$$c^{-2}u_{tt}^{(0)} - u_{xx}^{(0)} - \beta u_{txx}^{(0)} = \gamma (u^{(0)^2})_{tt} \,.$$
⁽⁹⁵⁾

Equation (95) is satisfied for $u^{(0)}$, since this is the solution to equation (48).

By equating the terms of order ε , we obtain the linearized Westervelt equation

$$c^{-2}u_{tt}^{(1)} - u_{xx}^{(1)} - \beta u_{txx}^{(1)} = 2\gamma (u^{(0)}u^{(1)})_{tx}$$

or alternatively in the operator form, with replacing $u^{(1)}$ for u,

$$\widetilde{\mathfrak{D}}_1 u = 0, \quad \widetilde{\mathfrak{D}}_1 = v^2 \partial_t^2 - \partial_x^2 - \beta \partial_{txx} - 2\gamma (u_{tt}^{(0)} \mathrm{id} + 2u_t^{(0)} \partial_t) \,. \tag{96}$$

As can be seen, equations (82) and (96) are exactly the same equations at the symbolic level, thereby eventually leading to the same ABCs. Thus, the para-differential approach to the construction of ABCs is equivalent to the asymptotic expansion method.

In order to para-linearize the Westervelt equation the para-differential approach uses the Taylor expansion with the assumption that the nonlinear function vanishes at zero. This means that in terms of the Taylor linearization of the right hand side $f(u) = \gamma(u^2)_{tt}$ of the Westervelt equation (43), f(u) vanishes at the reference solution $u^{(0)}$. Therefore, the following remark is valid.

Remark 3.3. The same assumption, the para-differential technique relies on, being introduced into the Taylor expansion applied to the right hand side of the Westervelt equation (43) gives the same result as the para-linearization thus making these approaches equivalent to each other. From the other hand, the para-linearization is equivalent to the

- asymptotic expansion as well as to the Taylor linearization, which, as we showed, prevents the offset term $\gamma \left(\left(u^{(0)} \right)^2 \right)$
- of being introduced into the absorbing boundary conditions. Therefore, we conclude that there do not appear to be

²⁹⁸ sufficient reasons to derive ABCs through the para-differential technique unless the coefficients have limited regularity.

Overall, we found that the para-differential technique is equivalent to both the asymptotic expansion of the Westervelt equation and to the linearization of its right hand side through the standard linearization according to the first order Taylor expansion with the assumption that the nonlinear function vanishes at the reference solution $u^{(0)}$.

³⁰² 3.4. Absorbing boundary conditions in 2-d via linearization and pseudo-differential calculus

³⁰³ In the spatially two dimensional situation the operator form of the Westervelt equation (43) reads as

$$\mathfrak{D}_1 u = 0, \quad \text{with } \mathfrak{D}_1 = \nu^2 \partial_t^2 - \partial_x^2 - \partial_y^2 - \beta \partial_{txx} - \beta \partial_{tyy} - 2\gamma u_t^{(0)} \partial_t \quad \text{in } (-\infty, 0) \times \mathbb{R},$$
(97)

where ν is defined by (50). Here, we proceed very similarly to the 1-d case, and consider pseudo-differential operators $A = A(x, y, t, D_y, D_t)$ and $B = B(x, y, t, D_y, D_t)$ with respect to time and tangential (i.e. y) direction, but the expansion is still with respect to powers of τ , so equations (51), (52) (with $A = A(x, y, t, D_y, D_t)$ and $B = B(x, y, t, D_y, D_t)$) remain the same, whereas (53), (54), (57) change to

$$v^{2}(i\tau)^{2} - (i\eta)^{2} - \beta(i\tau)\partial_{x}^{2} - \beta(i\tau)(i\eta)^{2} - 2\gamma u_{t}^{(0)}(i\tau) = (a+b)\partial_{x} + b_{x} - ab + R$$
(98)

with the correspondence $i\eta \leftrightarrow \partial_{y}$ and

$$a(x, y, t, \eta, \tau) \sim \sum_{j \ge 0} a_{1-j}(x, y, t, \eta, \tau), \quad |\tau| \to \infty,$$
(99a)

Igor Shevchenko, Barbara Kaltenbacher / Journal of Computational Physics 00 (2016) 1-27

309

$$b(x, y, t, \eta, \tau) \sim \sum_{j \ge 0} b_{1-j}(x, y, t, \eta, \tau), \quad |\tau| \to \infty,$$
(99b)

310 and

$$v^{2}(i\tau)^{2} - (i\eta)^{2} - \beta(i\tau)\partial_{x}^{2} - \beta(i\tau)(i\eta)^{2} - 2\gamma u_{t}^{(0)}(i\tau) = \sum_{j\geq 0} (a_{1-j} + b_{1-j})\partial_{x} + \sum_{j\geq 0} \partial_{x}b_{1-j} - \sum_{j\geq 0, k+l+n=j} \underbrace{\left(\frac{(-i)^{n}}{n!}\partial_{\tau}^{n}a_{1-k}\partial_{t}^{n}b_{1-l}\right)}_{O(\tau^{2-j})}, \quad k, l, n \geq 0,$$
(100)

respectively, where a_{1-j} and b_{1-j} are homogeneous functions of degree 1 - j in τ (and are additionally functions of $x, y, t, and \eta$). As in [19], in our derivations we rely on an assumption of the type $\eta \sim \tau$. Therewith, $\beta(i\tau)(i\eta)^2$ becomes a third order term that cannot be matched by the right hand side. Thus, in two space dimensions we already here arrived at the limitations due to the strong damping term (see also Remark 3.2 above), which we therefore omitted from now on by setting $\beta = 0$. Considering the $O(\tau^2)$ terms in (100) leads to

$$\begin{cases} v^2 (i\tau)^2 - (i\eta)^2 = -a_1 b_1, \\ a_1 + b_1 = 0. \end{cases}$$
(101)

³¹⁶ in place of (58), which results in

$$b_1 = -a_1 = \sqrt{\nu^2 (i\tau)^2 - (i\eta)^2} \,. \tag{102}$$

At this point, a fundamental difference to the 1-d case arises, since one has to approximate the square root

$$\sqrt{\nu^2(i\tau)^2 - (i\eta)^2} = \nu(i\tau) \sqrt{1 - \frac{\eta^2}{\nu^2 \tau^2}}$$

in order to derive practically applicable boundary conditions. We do so by a Taylor expansion whose order is adapted

319 to the order of the ABCs.

The calculations for a_0 , b_0 look exactly the same as in the 1-d case and yield

$$b_0 = -a_0 = -\frac{1}{2a_1} \left(ia_{1\tau} a_{1t} + a_{1x} - 2\gamma u_t^{(0)}(i\tau) \right)$$
(103)

321 i.e.

$$b_0 = -a_0 = -\frac{\nu_t}{2} \left(1 - \frac{\eta^2}{\nu^2 \tau^2} \right)^{-3/2} - \frac{\nu_x}{2\nu} \left(1 - \frac{\eta^2}{\nu^2 \tau^2} \right)^{-1} - \frac{2\gamma u_t^{(0)}}{2\nu} \left(1 - \frac{\eta^2}{\nu^2 \tau^2} \right)^{-1/2}.$$
 (104)

To obtain zero order boundary condition we use the zero order Taylor expansion

$$(1-x)^{1/2} \approx 1, \quad x := \frac{\eta^2}{\nu^2 \tau^2}$$

³²³ in (102) to have

$$\tilde{p}_1^0 = -\tilde{a}_1^0 = \nu(i\tau). \tag{105}$$

³²⁴ For our first order boundary condition we use the first order Taylor approximation

$$(1-x)^{1/2} \approx 1 - \frac{1}{2}x$$
, $(1-x)^{-3/2} \approx 1 + \frac{3}{2}x$, $(1-x)^{-1} \approx 1 + x$, $(1-x)^{-1/2} \approx 1 + \frac{1}{2}x$

for the terms that are nonlinear with respect to τ , η in (103) and (104). This yields the following symbols

$$\begin{split} \tilde{b}_1^1 &= -\tilde{a}_1^1 &= \nu(i\tau) \left(1 - \frac{\eta^2}{2\nu^2\tau^2} \right), \\ \tilde{b}_0^1 &= -\tilde{a}_0^1 &= -\frac{\nu_t}{2} \left(1 + \frac{3\eta^2}{2\nu^2\tau^2} \right) - \frac{\nu_x}{2\nu} \left(1 + \frac{\eta^2}{\nu^2\tau^2} \right) - \frac{2\gamma u_t^{(0)}}{2\nu} \left(1 + \frac{\eta^2}{2\nu^2\tau^2} \right). \end{split}$$

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Again we insert *u* itself for the a priori solution $u^{(0)}$ to arrive at the zero order ABC

$$\left(u_x + \sqrt{c^{-2} - 2\gamma u} \, u_t\right)\Big|_{x=0} = 0 \tag{106}$$

327 and at the first order boundary condition

$$\left(u_{xt} + \sqrt{c^{-2} - 2\gamma u} u_{tt} - \frac{1}{2\sqrt{c^{-2} - 2\gamma u}} u_{yy} - \frac{\gamma}{2\sqrt{c^{-2} - 2\gamma u}} \left(u_t - \frac{1}{\sqrt{c^{-2} - 2\gamma u}} u_x \right) u_t + \frac{\gamma}{2(c^{-2} - 2\gamma u)^{3/2}} \left(\frac{1}{2} u_t + \frac{1}{\sqrt{c^{-2} - 2\gamma u}} u_x \right) \int_0^{\infty} u_{yy} dt \right) \bigg|_{x=0} = 0,$$

$$(107)$$

where we have multiplied the symbols with $(i\tau)$ to obtain (107) or alternatively

$$\left(u_{xtt} + \sqrt{c^{-2} - 2\gamma u} u_{ttt} - \frac{1}{2\sqrt{c^{-2} - 2\gamma u}} u_{yyt} - \frac{\gamma}{2\sqrt{c^{-2} - 2\gamma u}} \left(u_t - \frac{1}{\sqrt{c^{-2} - 2\gamma u}} u_x \right) u_{tt} + \frac{\gamma}{2(c^{-2} - 2\gamma u)^{3/2}} \left(\frac{1}{2} u_t + \frac{1}{\sqrt{c^{-2} - 2\gamma u}} u_x \right) u_{yy} \right) \Big|_{x=0} = 0,$$

$$(108)$$

where we have multiplied the symbols with $(i\tau)^2$ to obtain (108).

330 **4. Discretization**

In this section we consider the space and time discretizations for problem (43)-(45) and how to couple the derived ABCs with the numerical methods used. Our focus is on the 2-d ABCs, since the 1-d boundary conditions use the same principle for coupling. For the space discretization we apply the finite element method with the standard setting of Sobolev spaces for evolution problems, while the time integration is done by the classical Newmark method.

For the weak formulation it is natural to use the space H^1 , then the resulting variational problem reads as follows: for given initial data $u(\cdot, t = 0) = u_0$, $u_t(\cdot, t = 0) = u_1$, find $u \in L^2(0, T; H^1(\Omega))$, $u_t \in L^2(0, T; L^2(\Omega))$ and $u_{tt} \in L^2(0, T; H^{-1}(\Omega))$ such that for all $\phi \in H^1$ and for all times $t \in (0, T)$

$$\left\langle c^{-2}u_{tt},\phi\right\rangle_{\Omega} + \left(\nabla u,\nabla\phi\right)_{\Omega} - \left(u_{n} + \beta u_{tn},\phi\right)_{\Gamma_{A}} - \left(\beta\nabla u_{t},\nabla\phi\right)_{\Omega} - \left(\gamma(u^{2})_{tt},\phi\right)_{\Omega} = \left(g(t) + \beta u_{tn},\phi\right)_{\Gamma_{N}}$$
(109)

with $\langle \cdot, \cdot \rangle_{\Omega}$ denoting the duality product on $H^1(\Omega) \times H^{-1}(\Omega)$ and (\cdot, \cdot) standing for L^2 -inner product.

The integration of the zero order ABC (106) into the weak formulation (109) is straightforward: one has to express the ABC in terms of u_n and substitute it into the boundary term

$$-(u_n + \beta u_{tn}, \phi)_{\Gamma_A}, \qquad (110)$$

341 which gives

$$(v(u)u_t + (v(u)u_t)_t, \phi)_{\Gamma_A}$$

³⁴² However, such a straightforward substitution is not applicable to the first order ABC (108). In this case, we use a ³⁴³ Lagrange multiplier (LM) based approach proposed in [49]. The main idea is to introduce the LMs $\lambda = -u_n$ and ³⁴⁴ $\kappa = u_t$ on the absorbing boundary Γ_A and recast the boundary integral (110) as

$$-(u_n + \beta u_{tn}, \phi)_{\Gamma_A} = (\lambda + \beta \lambda_t, \phi)_{\Gamma_A}, \qquad (\lambda, \phi)_{\Gamma_A} := \int_{\Gamma_A} \lambda \phi \ d\Gamma_A = \sum_{i=1}^l \int_{\Gamma_A^i} \lambda \phi \ d\Gamma_A^i, \qquad (111)$$

where Γ_A is assumed to be piecewise smooth and decomposed into *l* non-overlapping smooth subparts Γ_A^i .

To couple the first order boundary condition (108) and equation (109) we reformulate (108) in the weak form:

$$-\left(\lambda_{tt},\mu\right)_{\Gamma_{A}^{i}}+\left(\nu(u)\kappa_{tt},\mu\right)_{\Gamma_{A}^{i}}-\frac{\kappa_{\tau}\mu}{2\nu}\Big|_{\partial\Gamma_{A}^{i}}+\left(\kappa_{\tau},\left(\frac{\mu}{2\nu}\right)_{\tau}\right)_{\Gamma_{A}^{i}}-\left(\frac{\gamma\kappa_{t}}{2\nu}\left(\kappa+\frac{\lambda}{\nu}\right),\mu\right)_{\Gamma_{A}^{i}}+\theta u_{\tau}\mu\Big|_{\partial\Gamma_{A}^{i}}-\left(u_{\tau}\theta_{\tau},\mu\right)_{\Gamma_{A}^{i}}=0,\qquad(112)$$

where $\theta = \frac{\gamma}{2\nu^{3/4}} \left(\frac{\kappa}{2} - \frac{\lambda}{\nu}\right)$ and τ is the tangential derivative to Γ_A^i , and $\partial \Gamma_A^i$ denotes the endpoints of Γ_A^i , i = 1, 2, ..., l. 347 The boundary condition (112) holds for all test functions μ out of an appropriate test space defined on Γ_A^i . To get 348

rid of the terms on $\partial \Gamma_A^i$, we allow only for test functions μ being equal to zero on $\partial \Gamma_A^i$, i = 1, 2, ..., L. Using for μ 349 piecewise linear and continuous hat functions in $H_0^1(\Gamma_A^i)$, we end up with 350

$$-\left(\lambda_{tt},\mu\right)_{\Gamma_{A}}+\left(\nu(u)\kappa_{tt},\mu\right)_{\Gamma_{A}}+\left(\kappa_{\tau},\left(\frac{\mu}{2\nu}\right)_{\tau}\right)_{\Gamma_{A}}-\left(\frac{\gamma\kappa_{t}}{2\nu}\left(\kappa+\frac{\lambda}{\nu}\right),\mu\right)_{\Gamma_{A}}-\left(u_{\tau}\theta_{\tau},\mu\right)_{\Gamma_{A}}=0.$$
(113)

To obtain a more simple algebraic structure, we use dual LMs [56, 57]. We also require no continuity for the LMs, 351 since it would result in poor approximation properties. Thus, we apply the crosspoint modification of mortar finite 352 elements to define the basis functions of the LMs ansatz space. With each interior node of Γ_A^i we associate one basis 353 function. The ansatz space for the LMs differs from the test space for μ , and we are formally in a Petrov–Galerkin 354 setting. Note that by construction the dimension of the test and ansatz space is the same. 355

The algebraic formulation of the coupled problem (109), (113) can be expressed as a semi-discrete system of 356 nonlinear ordinary differential equations 357

$$\mathcal{A}(\mathbf{v}^{n+1})\ddot{\mathbf{v}}^{n+1} + \mathcal{B}(\mathbf{v}^{n+1})\mathbf{v}^{n+1} + C(\mathbf{v}^{n+1})\mathbf{v}^{n+1} = \mathcal{F}^{n+1},$$
(114)

with the vector of unknowns $\mathbf{v} = (\mathbf{u}, \lambda, \kappa)^{\mathrm{T}}$ and the terms 358

$$\mathcal{A} = \begin{pmatrix} c^{-2}\mathbf{M} - 2\gamma \widetilde{\mathbf{M}} & 0 & 0 \\ 0 & -\mathbf{D} & \widetilde{\mathbf{B}} \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{B} = \begin{pmatrix} \beta \mathbf{K} - 2\gamma \widetilde{\mathbf{M}} & \beta \mathbf{D}^{\mathrm{T}} & 0 \\ 0 & 0 & -\frac{\gamma}{2} \widetilde{\mathbf{K}} \\ -\mathbf{M} & 0 & 0 \end{pmatrix}, \quad C = \begin{pmatrix} \mathbf{K} & \mathbf{D}^{\mathrm{T}} & 0 \\ -\mathbf{P} & \mathbf{Q} & -\frac{\gamma}{2} \widetilde{\mathbf{D}} \\ 0 & 0 & \mathbf{M} \end{pmatrix}, \quad \mathcal{F} = \begin{pmatrix} \mathbf{f} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix},$$

where the right hand side f represents the Neumann boundary condition; M and K are the standard mass and stiffness 359 matrices, respectively. The other matrices are responsible for nonlinear terms and coupling between the Westervelt 360 equation and the ABC. 361

In order to approximate the system of equations (114) in time, the generalized α -method [12] is applied: 362

$$\dot{\mathbf{v}}^{n+1} = a_1 \mathbf{v}^{n+1} - \hat{\mathbf{v}}^n, \quad \ddot{\mathbf{v}}^{n+1} = a_2 \mathbf{v}^{n+1} - \hat{\mathbf{v}}^n, \quad \text{where}$$
(115)
$$\hat{\mathbf{v}}^n = a_1 \mathbf{v}^n + \frac{(1 - \hat{\alpha}_f)\hat{\gamma} - \hat{\beta}}{\hat{\beta}} \dot{\mathbf{v}}^n + \frac{(1 - \hat{\alpha}_f)(\hat{\gamma} - 2\hat{\beta})}{2\hat{\beta}} \Delta t \ddot{\mathbf{v}}^n, \quad \hat{\mathbf{v}}^n = a_2 \mathbf{v}^n + \frac{1 - \hat{\alpha}_m}{\hat{\beta}\Delta t} \dot{\mathbf{v}}^n + \frac{1 - \hat{\alpha}_m - 2\hat{\beta}}{2\hat{\beta}} \ddot{\mathbf{v}}^n$$

with the parameters $a_1 = (1 - \hat{\alpha}_f)\hat{\gamma}/(\hat{\beta}\Delta t)$, $a_2 = (1 - \hat{\alpha}_m)/(\hat{\beta}\Delta t^2)$, and Δt is a time step. In all computations we set 363 $\hat{\alpha}_m = \hat{\alpha}_f = 0, \ \hat{\beta} = 0.25, \ \hat{\gamma} = 0.5$, which results in the standard Newmark scheme [35] the application of which 364 to (114) yields 365

$$a_2 \mathcal{A}(\mathbf{v}^{n+1}) \mathbf{v}^{n+1} + a_1 \mathcal{B}(\mathbf{v}^{n+1}) \mathbf{v}^{n+1} + C(\mathbf{v}^{n+1}) \mathbf{v}^{n+1} = \mathcal{F}^{n+1} + \mathcal{A}(\mathbf{v}^{n+1}) \hat{\mathbf{v}}^n + \mathcal{B}(\mathbf{v}^{n+1}) \hat{\mathbf{v}}^n.$$
(116)

To solve the nonlinear system (116) we use the Newton method, demonstrating excellent convergence behavior 366 and robustness with respect to the choice of governing parameters in (43), acoustic source settings and ABCs. 367

5. Numerical results 368

369 In this part, we study the performance of the proposed absorbing boundary conditions in one and two space dimensions for different regimes of wave propagation. First, we analyzed the accuracy of ABCs derived with the 370 pseudo-differential and para-differential approaches in a one dimensional waveguide. Second, we considered a two 371 dimensional, horizontal waveguide with an inclined, artificial lateral wall and studied how the accuracy of the solution 372

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was influenced by the angle of incidence and the excitation frequency. Third, we carried out numerical experiments
 for the High Intensity Focused Ultrasound (HIFU) problem with settings typical for thermal ablation of tumors in the
 human liver and analyzed how intensively the solution was contaminated by reflected waves.

We denote the absorbing boundary conditions as $ABC_n^{d,o}$, where the superscripts d and o indicate the space dimension and the order of ABC, respectively, while the subscript *n* stands for the pseudo- (PS) or para-differential (PR) calculus based ABC, or the Engquist–Majda (EM) boundary condition, respectively. Here, by Engquist–Majda ABCs we mean those designed for the linear wave equation, so not taking into account the nonlinearity and the strong damping in the Westervelt equation.

In order to compare different ABCs, a reference solution u^* was computed in the domain $\Omega' \supseteq \Omega$, which is 381 large enough to prevent the solution in the restricted domain Ω from being polluted during the computations. Note 382 that u^* was computed for the same problem settings and physical parameters as u (the solution affected by reflected 383 waves) but in a larger computational domain. The studied ABCs were compared in terms of an l^2 -norm relative error 384 $\delta(u^*, u) = ||u^* - u||_2 / ||u^*||_2$, between the reference solution and the solution u distorted by reflected waves. We also 385 introduce a difference $\delta(u^*, u) = u^* - u$, which allows us to track reflected waves. In all numerical experiments the 38 number of finite elements per wavelength was set to be 50, and the time step was chosen in such a way as to have 20 387 time samples per time period for each of the frequencies $\omega = \{25 \text{ kHz}, 50 \text{ kHz}, 100 \text{ kHz}, 1 \text{ MHz}\}$. To induce a wave in 388 the domain, a monofrequency excitation of the form $u_n = \sin(2\pi\omega t)$ was used. The simulation time t and the initial 389 acoustic pressure amplitude were normalized to unity. The physical parameters in all numerical tests correspond to 390 those of human liver [28, 15]: $c = 1596 \text{ m} \cdot \text{s}^{-1}$, $\rho = 1050 \text{ kg} \cdot \text{m}^{-3}$, B/A = 6.8, $b = 2\alpha c^3/(2\pi\omega)^2$, with the acoustic 391 absorption coefficient $\alpha = 4.5 \text{ Np} \cdot \text{m}^{-1} \cdot \text{MHz}^{-1}$. 392

³⁹³ 5.1. ABC in 1-d

In this section, we compare ABC_n^{1,o}, with $o = \{0, 1\}$, $n = \{PS, PR, EM\}$ on a line segment $\Omega \in [0, 16 \text{ cm}]$ and study how the excitation frequency of the transducer influences the performance of the ABCs considered. The excitation u_n with one of the frequencies $\omega = \{25, 50, 100\}$ kHz was set at the point $\Gamma_N = 0$, while the ABC studied was prescribed at the point $\Gamma_A = 16 \text{ cm}$ (Fig. 1).



Fig. 1: General geometrical setup for the line segment domain Ω .

We present a series of snapshots of the reference solution u^* and the solution u affected by the boundary conditions ABC_n^{1,0}, o = {0, 1}, n = {PS, EM} in Fig. 2. As can be seen, for $t \in [0, 1]$, the difference between ABC_{PS}^{1,0} and ABC_{PS}^{1,1} is fairly small and slightly discloses itself only near the solution extrema. The same scenario is followed by the first order Engquist–Majda condition but only for $t \le 0.2$. However, as time advances the reflected waves start contaminating the solution. More insightful information on how the boundary conditions perform in time is given by the relative error δ presented in Fig. 3.

As can be seen from Fig. 3, the accuracy of the proposed ABCs does not significantly depend on the excitation frequency, although the relative error δ for the first order Engquist–Majda condition ABC^{1,1}_{EM} and the zero-order condi-404 405 tion $ABC_{PS}^{1,0}$ becomes somewhat higher in the low-frequency regimes. The first order conditions $ABC_{PS}^{1,1}$ and $ABC_{PR}^{1,1}$ 406 perform equally well at all frequencies studied. The behaviour of the boundary conditions $ABC_{PS}^{1,0}$ and $ABC_{PS}^{1,1}$ brings no surprise - the higher the order of the ABC is, the more accurate the solution becomes. The error δ , introduced 407 408 by ABC^{1,0}_{PS}, exhibits a very moderate growth at the initial stage of the simulation ($t \in [0.2, 0.6]$) with the maximum 409 reached at $t \approx 0.6$. For t > 0.6, the error moderately fluctuates around a mean value with no further growing. On the other hand, the first order condition ABC^{1,1}_{PS} demonstrates qualitatively the same behaviour as the zero order one, but on a much lower scale. The relative error δ also fluctuates around a mean, but these fluctuations are much smaller compared to those of ABC^{1,0}_{PS}. It is important to remark that the difference between ABC^{1,1}_{PS} and ABC^{1,1}_{PR} is virtually the same, indicating that the additional term $2\gamma u_t$ in ABC^{1,1}_{PR} (see the boundary condition (91) for detail) is of minor 410 411 412 413 414 importance. In contrast to the proposed ABCs, the first order Enquist-Majda condition is of much less accuracy. It 415



Fig. 2: Typical snapshots of the reference solution u^* and the solutions $u|_{ABC_{EM}^{1,1}}$, $u|_{ABC_{PS}^{1,0}}$, $u|_{ABC_{PS}^{1,0}}$ affected by reflected waves from the first order Engquist–Majda condition, zero and first order ABCs based on the pseudo-differential calculus, respectively. The excitation frequency is $\omega = 100 \,\mathrm{kHz}.$



Fig. 3: One dimensional waveguide. Relative error δ versus time t for different excitation frequencies ω and for the first (ABC^{1,1}_{EM}) order Engquist-Majda condition, zero (ABC^{1,0}_{PS}) and first (ABC^{1,1}_{PS}) order boundary conditions based on the pseudo-differential calculus, and the first order para-differential condition (ABC^{1,1}_{PS}). Note that the rectangular in the right down corner is a magnification of the lower part of the graph.

also has an initial growing trend for $t \in [0.2, 0.6]$, which is, however, much steeper than that of the conditions ABC^{1,0}_{PS}, 416 $ABC_{PS}^{1,1}$, and the fluctuations are significantly larger. 417

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We would like to draw the reader's attention to the resemblance between the error plots for $ABC_{PS}^{1,0}$ and $ABC_{EM}^{1,1}$: the local disturbance at t = 0.6 on both graphs (noticeable for $ABC_{EM}^{1,1}$, and barely perceptible for $ABC_{PS}^{1,0}$), as well 419 as the declined trend for t > 0.6. By analyzing the reflected waves for the boundary conditions ABC_n^{1,0} ($o = \{0, 1\}$, 420

 $n = \{EM, PS, PR\}$) we found that $\widetilde{\delta}\left(u^*, u\Big|_{ABC_{EM}^{1,1}}\right) \approx \widetilde{\delta}\left(u^*, u\Big|_{ABC_{PS}^{1,0}}\right)$ in the sense that their extrema evolve in a similar way 421

and appear essentially at the same instances in time (Fig. 4). Although $ABC_{EM}^{1,1}$ and $ABC_{PS}^{1,0}$ are quantitatively different, their qualitative resemblance is evident. In effect, such a similarity is not a coincide. These boundary conditions are very similar in form, and $ABC_{EM}^{1,1}$ can be derived analogously to $ABC_{PS}^{1,0}$ by taking $u^{(0)} = 0$ in the linearized Westervelt 422

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Fig. 4: One dimensional waveguide. Typical snapshots of the difference $\delta = u^* - u$ (vertical axis) between the reference solution u^* and the solution u distorted by reflected waves from the first (ABC^{1,1}_{EM}) order Engquist–Majda condition, zero (ABC^{1,0}_{PS}) and first (ABC^{1,1}_{PS}) order boundary conditions based on the pseudo-differential calculus, and the first order para-differential condition (ABC^{1,1}_{PS}).

equation (46). However, the boundary conditions $ABC_{PS}^{1,1}$ and $ABC_{PR}^{1,1}$ work differently and possess similarity with neither of the two mentioned.

427 5.2. ABC in 2-d

In this part we study how the boundary conditions with $ABC_n^{2,o}$, $o = \{0, 1\}$, $n = \{PS, PR, EM\}$ absorb ultrasound waves at different frequencies and angles of incidence in a two-dimensional horizontal acoustic waveguide and also analyze the performance of the ABCs for the High-Intensity Focused Ultrasound problem.

431 5.2.1. Acoustic waveguide

We consider a two-dimensional horizontal acoustic waveguide $\Omega \in [0, 8 \text{ cm}] \times [0, 18 \text{ cm}]$ and the excitation u_n with a frequency $\omega = \{25, 50, 100\}$ kHz set on the left boundary Γ_N of the domain Ω . The ABC studied was prescribed on the right boundary Γ_A , which is inclined to the horizontal axis at one of the angles $\alpha = \{75^\circ, 60^\circ, 45^\circ\}$ (Fig. 5).



Fig. 5: General geometric setup for the horizontal acoustic waveguide Ω .

A series of snapshots of the reference solution u^* and the solution affected by the boundary conditions $ABC_n^{2,o}$ (o = {0, 1}, n = {PS, EM}) are shown in Fig. 6. In this case, the situation is essentially the same as for the 1d waveguide. The Engquist–Majda condition of first order significantly pollutes the solution with reflected waves

- (Fig. 6(b)). The second order Engquist-Majda ABC outperforms the first order one, but the reflections are still very 438
- large (Fig. 6(c)). Per contra, the zero order condition $ABC_{PS}^{2,0}$ exhibits a much better performance and only introduces 439
- 440
- 441
- low-amplitude reflected waves into the solution (Fig. 6(d)). The first order conditions $ABC_{PS}^{2,1}$ and $ABC_{PR}^{2,1}$ demonstrate a considerable improvement and a very accurate solution compared to the conditions $ABC_{EM}^{2,1}$, $ABC_{EM}^{2,2}$ and $ABC_{PS}^{2,0}$ (Fig. 6(e)). We did not present the results for the boundary condition $ABC_{PR}^{2,1}$ derived via the para-differential approach, 442
- since, as in the one-dimensional case, it gives essentially the same accuracy as $ABC_{PS}^{2,1}$. 443
- The dependency of the ABCs, considered in this section, on the excitation frequency ω echoes that of the ABCs 444
- in 1-d case there is no considerable loss of accuracy when ω changes (Fig. 7). On the contrary, the incident angle α 445
- significantly affects the performance of the ABCs. As α decreases, so does the accuracy, and this effect is more pro-446
- nounced for the first and second order Engquist-Majda boundary conditions. The proposed ABCs are less influenced 447
- by the angle of incidence compared to the Engquist-Majda conditions and still give relatively accurate results even in 448
- low- α regimes. 449



Fig. 6: Typical snapshots of the solution in the 2-d waveguide with $\alpha = 75^{\circ}$ and $\omega = 100$ kHz: (a) the reference solution u^* ; and the solution u distorted by reflect waves from the boundary conditions (b) $ABC_{EM}^{2,1}$, (c) $ABC_{EM}^{2,2}$, (d) $ABC_{PS}^{2,0}$, (e) $ABC_{PS}^{2,1}$.



Fig. 7: Dependency of the relative error δ on the excitation frequency ω and the incidence angle α in the wo dimensional waveguide. Relative error δ versus time *t* for the first (ABC^{2,1}_{EM}) and second (ABC^{2,2}_{EM}) order Engquist–Majda conditions, and for the zero (ABC^{2,0}_{PS}) and first (ABC^{2,1}_{PS}) order boundary conditions based on the pseudo-differential calculus.

450 5.2.2. High-Intensity Focused Ultrasound problem

In this part, we studied the HIFU problem in which we used monofrequency excitation by a concave array of transducers, with an aperture of 20 mm and excitation frequency $\omega = 1.0$ MHz, located on the bottom of the domain Ω (Fig. 8). Such a transducer array shape allows to focus high intensity ultrasound waves on the desired place within the sonicated biotissue and create a local temperature increase to destroy tumor cells. On the rest of the boundary Γ_A we set the ABC studied. The configuration of the computational domain used as well as the transducer characteristics and the problem parameters are typical for numerical simulations of HIFU ablations of tumors.

⁴⁵⁷ The accuracy of ABCs for the HIFU problem is one of the most important issues, since in case of using inaccurate ⁴⁵⁸ ABCs reflected waves can significantly contaminate the acoustic pressure field, which, in turn, is used in the coupled ⁴⁵⁹ thermo-acoustic HIFU problem to compute the temperature distribution in the sonicated biotissue. The knowledge of ⁴⁶⁰ the temperature field determines the success of any HIFU therapy and therefore its distortion can lead to misinterpre-⁴⁶¹ tation of simulation results.

The reference solution u^* and the solution u influenced by reflected waves from the boundary conditions ABC_n^{2,0} (o = {0, 1}, n = {EM, PS}) at different characteristic time steps are shown in Fig. 9.



Fig. 8: General geometric setup for the high-intensity focused ultrasound problem.



Fig. 9: Snapshots of the solution for the HIFU problem: (a) the reference solution u^* ; and the solution u distorted by reflect waves from the boundary conditions (b) $ABC_{EM}^{2,1}$, (c) $ABC_{EM}^{2,2}$, (d) $ABC_{PS}^{2,0}$, (e) $ABC_{PS}^{2,1}$.

The difference between these boundary conditions is clearly visible. In particular, the second order Engquist– Majda ABC outperforms the first order one, especially in the focal spot, where the solution is affected the most by the

- reflected waves (Figs.9(b) and 9(c)). Interestingly that far off the focus the first order Engquist–Majda ABC seems to
- ⁴⁶⁷ perform even better than its second order version. However, overall the second order Engquist–Majda condition gives a better accuracy as opposed to the first order one.



Fig. 10: HIFU problem. Relative error δ versus time *t* for the first $(ABC_{EM}^{2,1})$ and second $(ABC_{EM}^{2,2})$ order Engquist–Majda conditions, and for the zero $(ABC_{PS}^{2,0})$ and first $(ABC_{PS}^{2,1})$ order boundary conditions based on the pseudo-differential calculus.

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The proposed ABCs of zero and first order demonstrate much more accurate results than the Engquist–Majda ABCs in both the focal zone and in the periphery of the computational domain (Figs.9(d) and 9(e)). Moreover, they

⁴⁷⁰ ABCs in both the focal zone and in the periphery of the computational domain (Figs.9(d) and 9(e) ⁴⁷¹ also show a much smoother behaviour in time, which is confirmed by the relative error δ (Fig. 10).

472 6. Conclusions

In this work we have proposed local in space and time absorbing boundary conditions for the Westervelt equation in one and two space dimensions. The derivation of the boundary conditions is based on the theory of pseudoand para-differential calculus, which has been applied to the construction of absorbing boundary conditions for the Westervelt equation in this work for the first time. We have found that both techniques lead to essentially the same absorbing boundary conditions in terms of computational efficiency and numerical accuracy.

We have studied different approaches to the linearization of the Westervelt equation (the Taylor linearization, asymptotic expansions, and the Bony para-linearization) and found that they are all equivalent if the Taylor linearization uses the same assumption as the para-linearization approach - the function vanishes at the reference solution.

All our numerical tests exhibit no instabilities, and demonstrate both the efficiency and effectiveness of the pro-481 posed boundary conditions. They are also attractive from the computational point of view due to their local character 482 and are easy to implement into existing numerical methods. The developed absorbing boundary conditions provide 483 quantitatively much better results than the classical first and second order Engquist-Majda conditions and can effi-484 ciently handle different regimes of wave propagation in a wide range of excitation frequencies and angles of incidence. 485 This shows that it pays off to take into account the nonlinearity as well as strong damping present in the Westervelt 486 487 equation also in the boundary conditions. It is also important to remark that the application of the self-adapting technique [49] to the proposed boundary conditions will result in further improvements. 488

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