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DATA-DRIVEN DISCOVERY OF A NONLINEAR WAVE EQUATION IN WEAK FORMULATION

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ABSTRACT

This paper deals with one of the subfields of physics-informed machine learning: data-driven discovery of partial differential equations. This work focuses on finite-amplitude sound propagation, i.e., nonlinear wave equations of the second-order approximation. Based on the principle of parsimony, we employ the sparsity promoting regression techniques to discover the governing equations. The training dataset was obtained by numerically solving the compressible Navier-Stokes equations. The investigated case involves the propagation of pressure pulses as travelling waves, leading to the discovery of the Westervelt equation. An algorithm trying to discover strong formulation of a partial differential equation suffers from low accuracy, due to the physical phenomena we are dealing with, i.e. local steep gradients. Improved accuracy was achieved when the problem is converted from strong formulation to a weak one. This benchmark study opens up opportunities for further discoveries in finite-amplitude sound propagation or findings linearizing transformations.

Keywords: *data-driven discovery, finite-amplitude sound propagation, weak formulation, Westervelt equation*

1. INTRODUCTION

Recently, physics-informed machine learning has gained attention. Here we focus on one of its subfields, the data-driven discovery of partial differential equations (PDEs – see e.g., [1–3]). In the field of finite-amplitude acoustics, the potential of equation discovery was shown in [4] on data obtained from numerically solved compressible Navier-Stokes equations. Based on Ockham's razor principle, the goal was to find a model sparse in terms included in the model. Hence, providing a closed library of candidate terms, one sparse regression methods (in this case LASSO [5]) is employed to re-discover the governing equations. However, the discovery of bulk losses turned out to be below the discrimination capability of the chosen method, since the losses were of order comparable to noise. Filtering the noise would not be a solution: steep derivatives that are by the nature of things present in the finite-amplitude acoustics would then diminish and the very essence of data would be lost. This issue could be overcome by converting finding PDEs from the strong formulation to a weak one. Benchmarking the PDE finder on known equations in finite-amplitude acoustics allows later for data-driven discovery or finding linearizing transformations.

This paper is organized as follows. In Sec. 2, the governing equations are introduced together with the numerical solver employed for obtaining the training dataset. Next, the discovery of the wave equation in weak formulation is described in Sec. 3. The results are presented and discussed in Sec. 4 and finally, the conclusions are drawn in Sec. 5.

2. GOVERNING EQUATIONS AND THEIR NUMERICAL SOLUTION

In this paper, we show a developed procedure for equation discovery on weakly nonlinear travelling waves. The training dataset has to be generated from equations as

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close as possible to conservation laws (or are the direct equivalent of conservation laws) to avoid including any bias. Throughout this work, we assume that the medium is a viscous, thermally conducting gas governed by the ideal gas state equation. The compressible Navier-Stokes equations can be rearranged as a set of convection-diffusion equations valid up to the third order changes, suitable for the finite-amplitude acoustics, as was shown by Červenka and Bednařík [6]. These equations can be put to a form convenient for numerical solution by introducing the non-dimensional mass density Λ and the non-dimensional momentum density Π:

$$\frac{\partial \Lambda}{\partial t} + \frac{\partial \Pi}{\partial x} = 0 \,, \tag{1}$$

$$\frac{\partial \Pi}{\partial t} + \frac{\partial}{\partial x}\left(\frac{\Pi^2}{\Lambda} + \frac{1}{\gamma}\Lambda^\gamma\right) = b\frac{\partial^2}{\partial x^2}\left(\frac{\Pi}{\Lambda}\right) \,, \tag{2}$$

with

$$b = \frac{1}{\rho_0 c_0 \ell}\left[\zeta + \frac{4}{3}\eta + \kappa\left(\frac{1}{c_V} - \frac{1}{c_p}\right)\right] \,, \tag{3}$$

$$\gamma = \frac{c_p}{c_V} \,, \qquad c_0 = \sqrt{\frac{\gamma p_0}{\rho_0}} \,, \tag{4}$$

where ℓ, ζ, η, κ, c_V and c_p denote the characteristic spatial dimension, the bulk and shear viscosities, the specific heat ratios at constant volume and pressure, respectively. The subscript 0 labels the ambient variables (measured in a quiescent, unperturbed medium).

The non-dimensional pressure can be recovered from the solution of the equations as [6]:

$$p = \frac{1}{\gamma}\Lambda^\gamma - b_p\frac{\partial}{\partial x}\left(\frac{\Pi}{\Lambda}\right) \,, \tag{5}$$

where $b_p = \kappa(1/c_V - 1/c_p)/\rho_0 c_0 \ell$. Finally, the dimensional pressure is then obtained as $\tilde{p} = p\rho_0 c_0^2$.

The equations (1)–(2) are cast in the convection-diffusion form. Due to their nonlinear nature leading to formation of shocks, it is necessary to employ a high-resolution scheme for numerical integration. In this paper we use the Kurganov-Tadmor scheme [7] with the OSPRE flux limiter [8]. Although the numerical viscosity introduced by the algorithm is not large and does not hinder key physical processes (in particular the wave steepening), it still plays a non-negligible role in the equation discovery described below.

3. DISCOVERY OF THE WAVE EQUATION

A key point of many equation discovery algorithms is the creation of a library of candidate terms [3]. In the classical (strong) formulation of the problem of partial differential equations, it is necessary to numerically evaluate partial derivatives from the training data. Since the input is often not smooth enough, this approach leads to a significant intensification of noise. Of course, there are a number of approaches to partially circumvent this problem (e.g., using Golay-Savitzky filtering). However, these run into a fundamental problem in the case of finite-amplitude acoustics: here, the occurrence of local steep gradients is not just an artifact of unfortunate data processing, but also a physical phenomenon itself [9, 10]. The ability to use an equation discovery procedure such that it bypasses the need to compute derivatives from the data is vital to advancing the field any further.

A simple and elegant solution is provided by the weak-PDE-LEARN algorithm by Stephany and Earls [11]. Its variant and adaptation to our field we present in this paper. The main idea is to convert the problem of finding PDEs from the strong formulation to a weak one. Slightly simplified: Instead of ensuring the correct matching of the differential terms in the infinitesimal neighborhoods of the selected spacetime points, we focus on verifying that the integrals of the candidate terms fit together for any appropriately chosen weight functions. In the following paragraphs we will go through this concept.

Let Ω denote the domain $\Omega \equiv [0, X] \times [0, T]$ (i.e. we consider one spatial dimension for which $x \in [0, X]$ and time $t \in [0, T]$). The underlying physical system has non-zero losses, so infinite steep shocks do not form in it. We can therefore safely assume that the acoustic pressure field $p(x, t)$ in the training data is well-behaved (i.e. it forms a compact, connected set with a Lipshitz continuous boundary).

In the following, we use the multi-index notation of the partial derivatives:

$$\mathrm{D}^{\alpha(m,n)}p \equiv \frac{\partial p^{m+n}}{\partial x^m \partial t^n} \,, \tag{6}$$

so for instance the d'Alembertian can be written as

$$\frac{\partial^2 p}{\partial t^2} - \frac{\partial^2 p}{\partial x^2} \equiv \mathrm{D}^{(0,2)}p - \mathrm{D}^{(2,0)}p \,. \tag{7}$$

If we assume that we are in the limit of weakly nonlinear acoustics, then it makes sense to look for equations in a form that presents only a correction to the linear (small-amplitude) wave equation. Hence, the equation is sought in the form:

$$\mathrm{D}^{(0,2)}p - \mathrm{D}^{(2,0)}p = \sum_i c_i \mathrm{D}^{\alpha_i} p^{s_i} \tag{8}$$

where c_i, α_i and s_i denote the multiplicative constant, the multi-index and the power of the i-th candidate term. For the purposes of this article, we only allow s to take integer values of 1 and 2 (i.e. either the terms linear in pressure or with a quadratic nonlinearity).

Now we multiply both sides of the equation (8) by the weight function $w_k = w_k(x,t)$ and integrate over the whole spacetime domain Ω:

$$\int_\Omega w_k \left(\mathrm{D}^{(0,2)}p - \mathrm{D}^{(2,0)}p\right)\,\mathrm{d}x\,\mathrm{d}t = \sum_i c_i \int_\Omega w_k \mathrm{D}^{\alpha_i} p^{s_i}\,\mathrm{d}x\,\mathrm{d}t\ . \tag{9}$$

In full generality, Eq. (9) shall hold for any weight function $w_k(x,t) \in \mathcal{C}_c^\infty$. Here we restrict the analysis to the family of bump functions of the form:

$$w_k(x,t) = \exp\left[\frac{\beta r^2}{(x-x_0)^2 + (t-t_0)^2 - r^2} + \beta\right] \tag{10}$$

if (x,t) lies within a ball of radius r centered around (x_0,t_0). Or $w_k(x,t) = 0$ otherwise. The required "k-th realization" is given by the choice of β, r, x_0 and t_0. If we allow only the bump centers (x_0,t_0) lying well inside the domain Ω (i.e. distant from the boundary $\partial\Omega$ by more than r), we can make use of the fact that $w_k = 0$ at $\partial\Omega$. Hence, by Green's lemma:

$$\int_\Omega w_k \mathrm{D}^{\alpha_i} p^{s_i}\,\mathrm{d}x\,\mathrm{d}t = (-1)^{|\alpha_i|}\int_\Omega p^{s_i}\mathrm{D}^{\alpha_i} w_k\,\mathrm{d}x\,\mathrm{d}t\ , \tag{11}$$

where $|\alpha_i(m,n)| = m+n$. See Fig. 1 for schematic depiction.

This is the important step as it allows to switch the differentiation from the data $p(x,t)$ to the analytically differentiable weight function w_k. For completeness, of course, the same procedure can also be used with the d'Alembertian on the left-hand-side of Eq. (9).

By repeating this procedure for each test function and each candidate term, we obtain a system of algebraic equations for the coefficients c_i:

$$A_{ki}c_i = b_k\ , \tag{12}$$

where

$$A_{ki} = (-1)^{|\alpha_i|}\int_\Omega p^{s_i}\mathrm{D}^{\alpha_i} w_k\,\mathrm{d}x\,\mathrm{d}t\ , \tag{13}$$

$$b_k = \int_\Omega p\left(\mathrm{D}^{(0,2)}w_k - \mathrm{D}^{(2,0)}w_k\right)\,\mathrm{d}x\,\mathrm{d}t\ . \tag{14}$$

Now we can simply solve this set with an appropriate sparsity-promoting technique in order to get the active terms in the wave equation and their coefficients. In this article we employed the Least-squares-post-Lasso algorithm (see e.g., [12] for details).

4. RESULTS & DISCUSSION

In this conference paper we will show only one application of the above procedure, namely the discovery of the equation for weakly nonlinear travelling waves. From the training data, we select only the spatio-temporal domain in which the Gaussian pulses propagate without interfering or being in contact with boundary conditions of any kind.

We use the results of 41 simulations for different pulse amplitudes and widths to provide statistics on the accuracy of the discovered wave equation for comparison with known analytical models. Candidate terms were assumed as follows:

$$\mathrm{D}^{(1,0)}p\ ,\quad \mathrm{D}^{(0,1)}p\ ,\quad \mathrm{D}^{(0,3)}p\ , \tag{15}$$

$$\mathrm{D}^{(1,1)}p\ ,\quad \mathrm{D}^{(2,0)}p^2\ ,\quad \mathrm{D}^{(0,2)}p^2\ . \tag{16}$$

Since these are corrections to the d'Alembert wave equation, we can also physically interpret the individual terms: In the first line it is various loss mechanisms (odd derivatives with real coefficients) and in the second line it is convection and nonlinearity.

In each simulation, 100 weight functions were used which made the system well-overdetermined. The centers of the bump functions were chosen randomly with

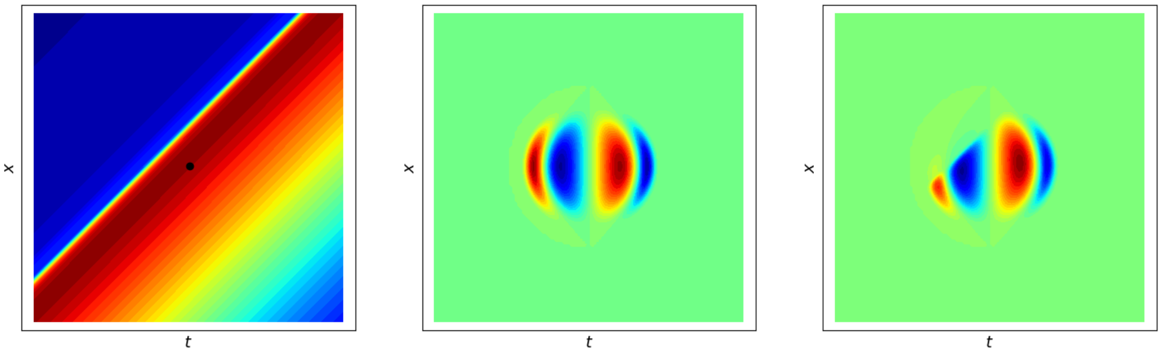

Figure 1. Illustrative depiction of manipulations in the PDE discovery algorithm in the weak form. Left: propagating pressure pulse $p(x,t)$ with a black dot denoting the center of the weight function. Middle: The 3rd time derivative of the weight function: $\mathrm{D}^{(0,3)}w_k(x,t)$. Right: an example of the integrand on the right-hand-side of Eq. (11): $p(x,t)\mathrm{D}^{(0,3)}w_k(x,t)$.

the constraint that the pressure at (x_0,t_0) must not be less than half of the maximum pressure in the dataset (otherwise some rows in the matrix A_{ki} could be trivial).

The resulting wave equation has the following form (for clarity, in the classical partial derivative notation):

$$\frac{\partial^2 p}{\partial t^2} - \frac{\partial^2 p}{\partial x^2} = (1.193 \pm 0.011)\,\frac{\partial^2 p^2}{\partial t^2} + + (0.001 \pm 0.000)\,\frac{\partial^2 p^2}{\partial x \partial t} + + (0.004 \pm 0.002)\,\frac{\partial^2 p^3}{\partial t^3}\,. \quad (17)$$

The first term on the right-hand side is the nonlinearity that corresponds to the Westervelt equation [9,10]. The value of its coefficient is within the confidence interval the same as the textbook value $(\gamma+1)/2$. Note that the relative width of the confidence interval is very small, so this is in fact a quite precise result.

The second term on the right-hand-side is quite small and virtually did not vary among the obtained results, which would suggest a systematic error of some sort. Basically, it is a correction to the unit wave propagation speed. It is very likely just a minor artifact of re-sampling.

The third term on the right-hand-side represents losses. Of all the differential order possibilities, the algorithm did indeed correctly select the one that would correspond to the thermoviscous attenuation in the bulk of the fluid. However, the coefficient is too big for the ideal gas and its confidence interval is quite large as well. Very likely, we are witnessing that the algorithm has correctly found a coefficient that matches the numerical viscosity of the solver [7]. This would explain both the coefficient's value and its variance, since the numerical viscosity in this case is proportional to the fourth spatial derivative and will therefore vary quite considerably for each initial condition.

It can be expected that the latter problem would not arise if the waves were propagating through a more lossy environment. Then the numerical viscosity of the solver could be small compared to the losses in the medium. As a trade-off, however, we would lose the advantage that the governing equations from which we take training data are close to the first principles, since the loss and nonlinearity parameters are often only measured in real fluids [9, 10].

5. CONCLUSIONS

In this work, we have demonstrated the advantages of discovering partial differential equations using the weak formulation. This approach proves effective for modeling the propagation of weakly nonlinear acoustic waves. In such cases, computing numerical derivatives — especially of second and third order — is often quite challenging and susceptible to noise amplification. In the weak form the discovery of nonlinear wave equations gets technically tractable and arguably more accurate.

Current efforts are focused on generalizing the approach to multiple spatial dimensions and to incorporate the interfering waves as well. At present, the work remains in the benchmarking phase, where the accuracy and robustness of the method are being systematically evaluated. Looking ahead, the promising applications lie in more realistic wave systems. These include, for example, the behavior of acoustic beams propagating through complex or heterogeneous media. There are even related machine learning techniques aimed at finding linearizing transforms.

6. ACKNOWLEDGMENTS

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