Accelerating numerical methods for

nonlinear acoustics using nested meshes

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The numerical simulation of nonlinear ultrasound is important in the treatment planning for high-intensity focused ultrasound (HIFU) therapies in the abdomen. However, the large domain sizes and generation of higher harmonics at the focus make these problems extremely computationally demanding. Numerical methods typically employ a uniform mesh fine enough to resolve the highest harmonic present in the problem, leading to a very large number of degrees of freedom. This paper proposes a more efficient strategy in which each harmonic is approximated on a separate mesh, the size of which is proportional to wavelength of the harmonic. The increase in resolution required to resolve a smaller wavelength is balanced by a reduction in the domain size. This nested meshing is feasible owing to the increasingly localised nature of higher harmonics near the focus.

Numerical experiments are performed for HIFU transducers in homogeneous media in order to determine the size of the meshes required to accurately represent the harmonics. In particular, a fast *volume potential* approach is proposed and employed to perform convergence experiments as the computation domain size is modified. This approach allows each harmonic to be computed via the evaluation of an integral over the domain. Discretising this integral using the midpoint rule allows the computations to be performed rapidly with the FFT. It is shown that at least an order of magnitude reduction in memory consumption and computation time can be achieved with nested meshing.

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1 I. INTRODUCTION

High-intensity focused ultrasound (HIFU) is a non-invasive tumor ablation therapy in 22 which acoustic waves are focused at a target location, thereby elevating the temperature sufficiently to destroy the tumor tissue. Tissue death can be caused directly via thermal ablation, or via other mechanisms such as cavitation (Izadifar et al., 2017; Vlaisavljevich 25 et al., 2013). In the thermal ablation setting, which is the focus of this article, the peak acoustic pressure is often between 1 and 10 MPa, at which linear acoustic theory is no longer accurate. Indeed it has been observed that the contributions from nonlinear effects can 28 increase the temperature at the focal point by an additional 20%, thus substantially reducing the time required for ablation when compared to simulations using linear theory (Solovchuk et al., 2014). Furthermore, the location of the focus in the nonlinear regime is often shifted 31 relative to that predicted by the linear theory (Camarena et al., 2013). To simulate the nonlinear acoustic field, a popular model is the Westervelt equation, which incoporates a quadratic pressure term. Numerically solving the Westervelt equation in a HIFU setting is computationally challenging since the domains are large compared to the smallest wavelength present. 36

To put into context the scale of the computational problems presented by HIFU, consider
a bowl-shaped HIFU transducer with radius 7.5cm and geometric focal length 15cm operating at 1.1MHz. Transducers of this size are suitable for deep-seated tumors, located in
the liver, for example. A simulation domain spanning the face of the bowl and extending to
the focal region is approximately 100 wavelengths across in each dimension. If there are five

harmonics present in the nonlinear field, then this is five hundred wavelengths at the fifth harmonic. In order to obtain a reasonable accuracy level, we can assume that at least six degrees of freedom (DOF) per wavelength are required (Marburg, 2008). Then to simulate this problem in three dimensions, we would require 27 billion degrees of freedom. Handling

such a large system presents an enormous computational load in terms of memory and time.

There has been a great deal of research effort aimed at reducing the computational cost of nonlinear HIFU simulations. Much of this work employs at least one simplifying assumption, such as axisymmetry, one-way wave propagation, or the parabolic approximation (see (Gu and Jing, 2015) for a review). The most popular methods for solving the original Westervelt equation (or equivalent) are the finite-difference time-domain method (Solovchuk et al., 2013) (FDTD) and the k-space pseudospectral method (Treeby et al., 2012) (KSPS). Although powerful techniques, these full-wave solvers can still yield simulation times in excess of a day for realistic problems when run on a large cluster (Jaros et al., 2016).

In this paper, we set out to improve upon the meshing strategies employed in the popular full-wave solvers, namely uniform meshes resolved according to the wavelength of the highest harmonic. Such a meshing approach is inefficient since the higher harmonics are localised around the focus, therefore the extremely fine mesh far away from the focus is likely overkill. It seems intuitive that a mesh that is gradually refined as the focus is approached would be sensible, but at what rate? And what saving can one expect to achieve? Here, we address these questions via numerical experimentation on realistic HIFU transducers taken from (Sonic Concepts, Accessed: 2020-08-19).

In order to perform these experiments efficiently, we consider a simplified setting in 63 which the propagation medium is homogeneous and the signal is assumed to have harmonic time dependence. Under the time-harmonic assumption, the full-wave Westervelt equation reduces to a series of inhomogeneous Helmholtz equations, one for each harmonic present in the field (as in, e.g., (Du and Jensen, 2013; Soneson, 2017)). Furthermore, since we consider a homogeneous medium, each Helmholtz equation is exactly solved by the evaluation of the appropriate volume potential integral (Costabel, 2015). Therefore, for each harmonic in the field, we look at the convergence of the volume potential as the domain of integration is increased. In order to efficiently evaluate the volume potential, we discretise the domain over 71 a uniform voxel mesh, which allows the summation (i.e., the discrete form of the integration) 72 to be performed rapidly using the fast-Fourier transform (FFT). This is an extremely efficient technique for computing high-order harmonics in a homogeneous medium and its application in this area is, to the best of the authors' knowledge, novel.

For numerical investigations with different transducer configurations and within two different media (water and liver), we deduce that (for the configurations considered) in order to
perform accurate computations of the second harmonic, the computation domain must extend all the way back to the transducer, however may be contracted slightly in the transverse
direction. For the third and higher harmonics, the computation domain may be contracted
in both the axial and transverse directions, thus leading to substantial computational savings. In fact, we demonstrate that an accurate approximation (less than 1% relative error)
may be obtained while contracting the width and length of the domain in proportion to the
wavelength of the harmonic. Thus the number of cells in every mesh is roughly equal. This

amounts to a reduction in the number of DOF by a factor of approximately $(n/2)^3$, where n is the number of harmonics being computed.

In practice, this leads to a series of nested meshes, each at the resolution required for the
appropriate harmonic and all with the same number of voxels. To perform computations for
higher harmonics, solutions from lower harmonics are interpolated onto the finer meshes. We
outline an algorithm for this more efficient computation of all the harmonics in Section VI
and examine its performance.

The layout of the paper is as follows. Section II outlines the mathematical model we 92 employ for our HIFU setup. In particular we consider the Westervelt equation and review how it reduces to a series of Helmholtz equations under the time-harmonic assumption. We further simplify the equations via an assumption of weak nonlinearity, which is valid for a large range of HIFU transducer settings. In Section III we describe how, in the homogeneous domain case, the Helmholtz equations are solved exactly via volume potentials. It is then described how these volume potentials are efficiently approximated using a voxelised discretisation approach. This leads to the discrete versions of the volume potentials having block-Toeplitz form; thus the potentials may each be evaluated using a single fast 100 matrix-vector product with the FFT. Section III B discusses our model for the time-harmonic 101 bowl-shaped transducer. Section IV presents a validation of our approach by comparing 102 to simulations performed with the HITU Simulator MATLAB toolbox (Soneson, Accessed: 103 2020-05-06, 2017). In Section V we perform convergence tests for each of the harmonics 104 for a range of problem setups. We present our findings on the rates of convergence of the 105 approximation as the domain is increased and present a rule of thumbs for designing the meshes to ensure each harmonic is accurately approximated. In Section VI we present how
the hierarchy of meshes is used in practice with our volume potential approach, including
the interpolation of approximations between the meshes. Here we present some performance
details for this three-dimension full-wave approach on a single workstation. Finally, in Section VII we present our conclusions and discuss the relevance of this work to numerical
techniques for HIFU, in particular finite-element methods, volume- and boundary-integral
equation methods, and coupled finite-element/boundary-element methods.

114 II. NONLINEAR ACOUSTICS IN THE FREQUENCY DOMAIN

Acoustic fields produced by HIFU transducers are commonly modelled by the Westervelt equation (Hamilton *et al.*, 1998):

$$\nabla^2 p - \frac{1}{c_0^2} \frac{\partial^2 p}{\partial t^2} - \frac{2\alpha_0}{c_0^{1-\eta}} \frac{\partial}{\partial t} \left(-\nabla^2 \right)^{\eta/2} p = -\frac{\beta}{\rho_0 c_0^4} \frac{\partial^2 p^2}{\partial t^2},\tag{1}$$

where p is the acoustic pressure, c_0 is the speed of sound, ρ_0 is the medium density, β the non-linearity parameter, and α_0 and η are medium specific attenuation parameters. The fractional Laplacian appearing in (1) was first introduced in (Chen and Holm, 2004) in order to incorporate frequency dependent power law attenuation. More specifically, in the frequency domain, it generates a complex wavenumber of the form

$$k = \frac{\omega}{c_0} + i\alpha; \quad \alpha = \alpha_0 |\omega|^{\eta},$$
 (2)

for $\alpha_0 |\omega|^{\eta-1} c_0 < 0.1$ (Szabo, 1994), where ω is the angular frequency of the transducer.

The power law exponent is typically in the range $1 \le \eta \le 2$. We note that this power law attenuation can also be incorporated via a temporal convolution, as was originally proposed

in (Szabo, 1994); we refer the reader to (Treeby and Cox, 2010) for a review of power law attenuation techniques.

In this article, we assume that the operation time of the transducer is long when compared to the period of the signal. Therefore, the total acoustic pressure can be written as the following sum over harmonics (as in (Du and Jensen, 2013; Soneson, 2017)):

$$p(\mathbf{x},t) = \operatorname{Re}\left\{\sum_{n=1}^{\infty} \left(p_n(\mathbf{x})e^{-in\omega t} + p_n^*(\mathbf{x})e^{in\omega t}\right)\right\},\tag{3}$$

where * denotes complex conjugation. Many numerical schemes in the literature consider the time-harmonic form (3), e.g., (Campos-Pozuelo *et al.*, 1999; Du and Jensen, 2013; Soneson, 2017; van 't Wout *et al.*, 2015), likely owing to the distinct advantages of a frequency domain approach:

- the challenging task of choosing/developing an efficient time stepping scheme can be avoided;
- arbitrary frequency-dependent attenuation power laws can be easily incorporated

 (whereas in the time domain one has to contend with the fractional Laplacian);
- methods such as the boundary element method and volume integral equation method,
 can be applied directly;
- the computation regions for higher harmonics can be reduced, thereby making simulations more efficient.
- 142 It is this final point that we study in this article.
- The form (3) is not well suited for substitution into (1) since the right-hand of (1) requires the computation of a product. For such a product, expressions in which real or

imaginary parts are required to be taken lead to cumbersome algebra. Therefore, it is more straightforward to use the following expression, which is equivalent to (3):

$$p(\mathbf{x},t) = \frac{1}{2} \sum_{n=1}^{\infty} \left(p_n(\mathbf{x}) e^{-in\omega t} + p_n^*(\mathbf{x}) e^{in\omega t} \right). \tag{4}$$

Substituting (4) into (1) and matching coefficients of $e^{-in\omega t}$ for $n \geq 1$ yields

$$\nabla^2 p_n + k_n^2 p_n = \frac{\beta \omega^2}{2\rho_0 c_0^4} n^2 \sum_{m=1}^{\infty} p_m (p_{n-m} + 2p_{m-n}^*), \tag{5}$$

for $n=1,2,\ldots$, where $p_n=0$ for $n\leq 0$, and the complex wavenumbers are defined as

$$k_n = \frac{n\omega}{c_0} + i\alpha(n\omega). \tag{6}$$

The equations (5) can be further simplified by neglecting small terms on the right-hand side, which is appropriate in the weakly nonlinear case, as was considered in, e.g., (Du and Jensen, 2013). Specifically, we neglect all terms $p_i p_j$ and $p_i p_j^*$ for which i + j > n, for n = 1, 2, ..., thus giving

$$\nabla^2 p_n + k_n^2 p_n = \frac{\beta \omega^2}{2\rho_0 c_0^4} n^2 \sum_{m=1}^{n-1} p_m p_{n-m}.$$
 (7)

This is a cascade of inhomogeneous Helmholtz equations in which each right-hand side is a combination of products of lower harmonics. Therefore, we can solve the equations sequentially, starting from n=1.

We note that the assumption of weak nonlinearity is valid for a wide range of HIFU applications for thermal ablation. However, for extremely high focal pressures such as those sometimes encountered in lithotripsy, where pressures much higher than 20MPa can be seen, the terms neglected above become significant (Izadifar *et al.*, 2017). Therefore, a modified approach would be required, however we do not consider this case here.

161 III. VOLUME POTENTIALS

The equations (7) are each of the general form

$$\nabla^2 u + k^2 u = f(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3.$$
 (8)

Via Green's theorem (see, e.g., (Colton and Kress, 2013; Costabel, 2015)) it can be seen that the following volume potential satisfies (8):

$$u(\mathbf{x}) = -\int_{\mathbb{R}^3} G_k(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}, \quad \mathbf{x} \in \mathbb{R}^3,$$
 (9)

where G_k is the fundamental solution to the Helmholtz equation,

$$G_k(\mathbf{x}, \mathbf{y}) = \frac{e^{ik|\mathbf{x} - \mathbf{y}|}}{4\pi |\mathbf{x} - \mathbf{y}|}, \quad \mathbf{x} \neq \mathbf{y}.$$
 (10)

We note that the integral in (9) is over an infinite domain, however in practice we replace this with a finite domain of integration, D. So we have that

$$u(\mathbf{x}) = -\int_{D} G_{k}(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y} + \varepsilon(D), \quad \mathbf{x} \in D \subset \mathbb{R}^{3},$$
(11)

where $\varepsilon(D)$ an error incurred by the introduction of a finite integration domain. Since the HIFU field is highly focused, a sensibly chosen finite D will yield a negligibly small error.

It is the purpose of this article to investigate how small D can be made whilst still yielding accurate approximations to u.

For clarity, we write out this integral representation (11) for each of the first five harmonics:

$$p_2(\mathbf{x}) = -\frac{2\beta\omega^2}{\rho_0 c_0^4} \int_{D_2} G_{k_2}(\mathbf{x}, \mathbf{y}) p_1^2(\mathbf{y}) d\mathbf{y}, \tag{12}$$

$$p_3(\mathbf{x}) = -\frac{9\beta\omega^2}{\rho_0 c_0^4} \int_{D_3} G_{k_3}(\mathbf{x}, \mathbf{y}) p_1(\mathbf{y}) p_2(y) d\mathbf{y},$$
(13)

$$p_4(\mathbf{x}) = -\frac{8\beta\omega^2}{\rho_0 c_0^4} \int_{D_4} G_{k_4}(\mathbf{x}, \mathbf{y})(p_2^2(\mathbf{y}))$$

$$\tag{14}$$

$$+2p_1(\mathbf{y})p_3(\mathbf{y}))\mathrm{d}\mathbf{y},\tag{15}$$

$$p_5(\mathbf{x}) = -\frac{25\beta\omega^2}{\rho_0 c_0^4} \int_{D_5} G_{k_5}(\mathbf{x}, \mathbf{y})(p_1(\mathbf{y})p_4(\mathbf{y})$$

$$+ p_2(\mathbf{y})p_3(\mathbf{y}))\mathrm{d}\mathbf{y},\tag{16}$$

where we have introduced the domains D_i , i=2,3,..., appropriate sizes of which are to be determined. In a homogeneous medium, the first harmonic p_1 is merely the incident field generated by the transducer, which we can compute anywhere in \mathbb{R}^3 . Note finally that the Green's functions in each of (12)-(16) possess the appropriate wavenumber for that harmonic, k_n , for n=2,3,4,5.

A. Efficient computation of the volume potential

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HIFU problems are reknowned for their challenging high-frequency nature, with domain sizes up to hundreds of wavelengths in each of the three dimensions. Therefore, the (singular) integrals in (12)–(16) are potentially enormously expensive to approximate.

We choose the integration domains D_i to be cuboidal in shape and to be discretized into uniform voxel grids $\mathcal{V}(D_i)$ so that the discrete form of the integral operator becomes a Toeplitz matrix. A Toeplitz matrix of dimension N has the property that it may be embedded in a circulant matrix of dimension 2N, with which a matrix-vector product can be computed with $\mathcal{O}(2N \log 2N)$ complexity using the fast-Fourier transform (FFT); see, e.g., (Groth *et al.*, 2020) for more details.

For the voxels in which the Green's function's singularity is located, we approximate the integral by the integral over a sphere of radius a, chosen such that the sphere's volume is equal to that of the voxel. The Jacobian of the transformation to spherical coordinates cancels the singularity in the Green's function. In the non-singular voxels we approximate the volume potential integral by the midpoint rule. This gives us the simple quadrature rule

$$\int_{V_{j}} G(\mathbf{x}_{i}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}$$

$$= \begin{cases}
\frac{1}{k^{2}} \{e^{ika}(1 - ika) - 1\} f(x_{j}), & \mathbf{x}_{i} \in V_{j}, \\
(\delta x)^{3} G(\mathbf{x}_{i}, \mathbf{x}_{j}) f(\mathbf{x}_{j}), & \mathbf{x}_{i} \notin V_{j},
\end{cases} \tag{17}$$

for i, j = 1, ..., N, where N is the number of voxels in the grid and δx is the side length of each voxel V_j . This is reminiscent of the 'discrete dipole approximation' often used in electromagnetic scattering calculations (Draine and Flatau, 1994). One can choose to opt for a more sophisticated quadrature rule here, however, this simple approach suffices for our purposes.

B. HIFU incident field

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In a homogeneous medium there is no scattering and therefore the first harmonic, p_1 , can be obtained directly from an appropriate model of the time-harmonic field generated by the HIFU source. In this paper, we consider bowl-shaped ultrasound transducers, which are designed to focus acoustic energy at a prescribed location, typically the centre of curvature of the bowl. More specifically, we consider for simplicity a single-element bowl-shaped transducer and discretise the surface using a Rayleigh integral type approach described below. We note that we are not exploiting symmetries in our approach and therefore more sophisticated multi-element transducer arrays, such as those in (Gavrilov and Hand, 2000; Gélat et al., 2011), can be incorporated in a straightforward manner.

To discretise the surface of the bowl transducer, we use evenly spaced points following (Deserno, 2004). At each of the evenly spaced point we place a monopole source, the expression for which is given by (10). Summing over the monopole sources gives the (unnormalised) first harmonic at any $\mathbf{x} \in \mathbb{R}^3$ as

$$\tilde{p}(\mathbf{x}) = \frac{A}{n_{\rm p}} \sum_{i=1}^{n_{\rm p}} G_k(\mathbf{x}, \mathbf{r}_i), \tag{18}$$

where $n_{\rm p}$ is the number of points, ${\bf r}_i$ are their locations on the bowl, and A is the total surface area of the bowl.

We note that in (18) no amplitude has been specified for the monopole sources. We instead choose to normalise the field to produce a prescribed total radiated power, Π, which is obtained by integrating the intensity over a sphere surrounding the source (Kinsler *et al.*, 1999). For a bowl-shaped transducer, the field is directed, so rather than integrating over a sphere, it suffices to integrate over a disc covering the open end of the bowl. This can be written as

$$\Pi(p) = \frac{1}{2\rho_0 c_0} \int_0^{2\pi} \int_0^R p^2(r, \theta) dr d\theta,$$
 (19)

where R is the outer radius of the bowl. Thus, the normalised first harmonic to yield a prescribed radiated power Π_0 is given as

$$p_1(\mathbf{x}) = \sqrt{\frac{\Pi_0}{\Pi(\tilde{p})}}\tilde{p}.$$
 (20)

In our experiments, we take $n_{\rm p}=4096$. Such a large value was required to avoid undesired interference patterns between the bowl and focus.

The two bowl transducer geometries considered in this article are taken from the Sonic Concepts website (Sonic Concepts, Accessed: 2020-08-19) and are detailed in Tab. I. Two

<i>j</i>	f_0 (MHz)) l (mm)	R (mm)	r (mm)
H101	1.1	63.2	64	0
H131	1.1	35	33	0

TABLE I. Operating frequencies and geometrical parameters of bowl transducers considered, taken from (Sonic Concepts, Accessed: 2020-08-19). The geometrical parameters are the geometric focal length l, the outer radius R, and the inner radius r. These can also be seen depicted in Fig. 1.

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propagation media are considered throughout: water and liver. The acoustic parameters for these are detailed in Tab. II.

C. How many points per wavelength?

Before deploying our scheme to compute high-order harmonics, it is necessary to understand the convergence rate as the mesh is refined, thereby enabling an adequate resolution

	$ ho_0$	$({\rm kg/m^3})$	c	(m/s)	β	α_0	η	(dB/m)
Water		1000		1480	3.5	0.2		2
Liver		1060		1590	4.4	90.0		1.1

TABLE II. Relevant medium parameters for water and liver at 1MHz (Azhari, 2010; Duck, 2013). The parameters α_0 and η pertain to the absorption power law in (2).

to be chosen for later investigations. In this article, we focus on achieving approximations with relative L^2 errors close to 1%.

To determine the convergence rate, we consider computing the second harmonic generated by the H131 transducer in liver, using equation (12). The configuration of the transducer is shown in Fig. 2; the bowl transducer is located at the origin and is directed along the x-axis. For the integration domain D_2 in (12) we take the white box in Fig. 2. This box is illustrated with detailed dimension definitions in Fig. 1. The domain D_2 is defined as

$$D_2 = [l - L, l + d] \times [-R, R] \times [-R, R], \tag{21}$$

where d is the distance of interest beyond the focus, l is the geometric focal length, and Rthe outer radius (see Fig. 1). The length L is defined as $L = \sqrt{l^2 - R^2} - \epsilon$ with ϵ chosen as a
small displacement from the bowl in order to avoid the singularity in the Green's functions
at the bowl's surface; we take $\epsilon = 0.1$ mm. The total radiated power of the transducer is set
as $\Pi_0 = 100$ W and the operating frequency is $f_0 = 1.1$ MHz.

The volume potential in (12) is computed using the method outlined in Section III A with increasingly refined voxel meshes. Specifically, we build meshes with voxel dimension

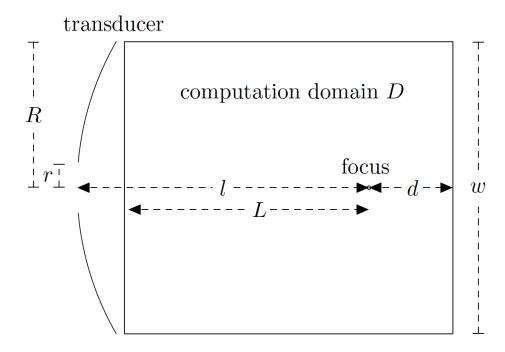


FIG. 1. Description of a generic computation domain D with length L+d and width (and depth) w.

 $\delta x = \lambda/(2n_w)$, where $\lambda = c/f_0$ is the fundamental wavelength and n_w is the 'number of voxels per wavelength'. The factor 2 in the denominator is to account for the fact that we are computing a field with wavelength $\lambda/2$, i.e., the second harmonic. The values of n_w considered are from 4 to 20, and a reference solution, denoted p_2^r , is computed using $n_w = 35$.

For each value of n_w , the relative L^2 -error of the field p_2 along the x-axis is computed; this is defined as

Error =
$$\frac{||p_2 - p_2^r||}{||p_2^r||} \times 100\%,$$
 (22)

where $||\cdot||$ denotes the L^2 -norm along the x-axis, i.e.,

$$||p_2|| := \left(\int_{l-L}^{l+d} |p_2(x)|^2 dx \right)^{1/2}.$$
 (23)

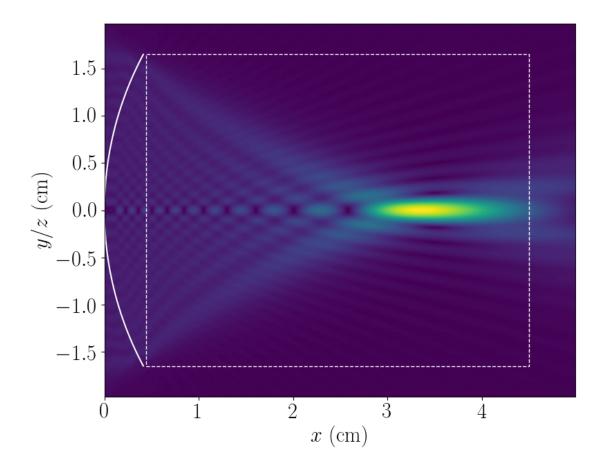


FIG. 2. Magnitude of the first harmonic generated by the H131 transducer in liver. The bowl transducer is represented by the arc at the far left. The dashed white line outlines the computation domain D_2 used to compute the second harmonic shown in Fig. 4.

We approximate the integrals in (22) using the midpoint rule with the mesh nodes of the reference solution, p_2^r , being used as the quadrature nodes.

The convergence results are shown in Figure 3. As is to be expected from the midpoint rule, quadratic convergence is obtained. From the graph we can read off that an error smaller than 1% is achieved with $n_w > 5$. Therefore we choose to take $n_w = 6$ for all harmonics in the experiments in the remainder of the article. The approximation to the second harmonic

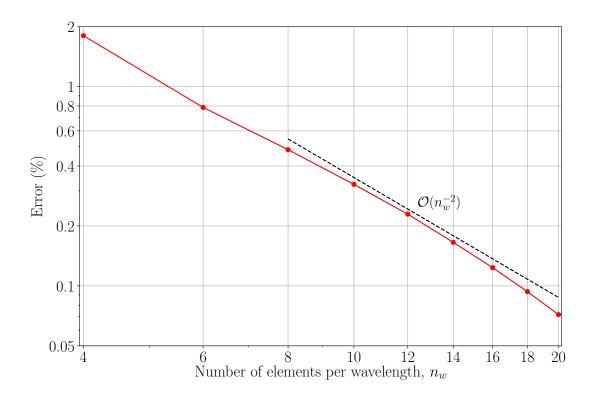


FIG. 3. The convergence of the quadrature rule for the computation of the second harmonic via (12). The convergence rate is quadratic in n_w and an error of smaller than 1% is achieved with $n_w > 5$.

with $n_w = 6$ is shown in Fig. 4 and can be seen to be indistinguishable from the reference solution.

260 IV. VALIDATION OF NUMERICAL SCHEME

To validate our approach for the computation of higher harmonics via the evaluation of the volume potentials in (12)-(16), we present a qualitative comparison to approximations obtained using *HITU Simulator* (Soneson, Accessed: 2020-05-06). HITU simulator is

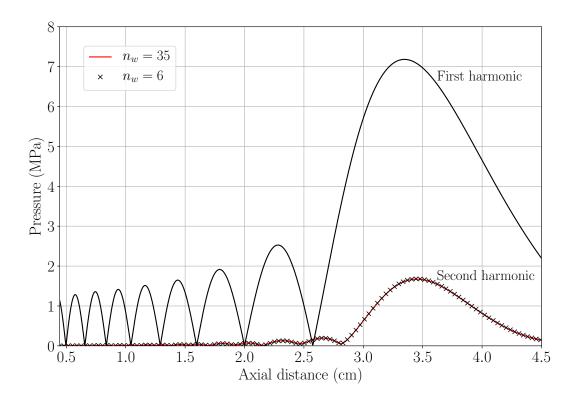


FIG. 4. The first and second harmonics along the x-axis for the H131 transducer in liver. With 6 voxels per wavelength the approximation to the second harmonic is indistinguishable from the reference solution.

an open-source MATLAB implementation of the high-order parabolic approximation to the axisymmetric Westervelt equation, i.e., the wide-angle Khokhlov-Zabolotkaya-Kuznetsov (WAKZK) equation. The method is detailed by the author of HITU simulator in (Soneson, 2017). The assumption of axisymmetry allows the dimension of the problem to be reduced by one and hence facilitates rapid simulations.

We consider two configurations:

1. H131 transducer at output power 50W in water;

2. H101 transducer at output power 100W in liver.

observe good qualitative agreement with the approximations obtained using HITU simulator 273 in the region around the focus, whereas towards the transducer the two methods disagree. 274 This is due to the parabolic assumption made in the derivation of the WAKZK equation, 275 which is only accurate when sufficiently far from the transducer. The volume potential 276 method on the other hand approximates solutions to the Westervelt equation so can be taken 277 to be accurate in this 'near field' region. Indeed, the computation of the first harmonic in 278 our approach, as outlined in Section IIIB, is equivalent to a Rayleigh integral method. 289 We observe that the volume potential method predicts a slightly larger amplitude for the 282 first and second harmonics than HITU simulator, but the third, fourth and fifth harmonics are almost identical. The two examples considered have considerably different attenuation 284 power law parameters, thus the strong agreement with HITU simulator for both examples 285 demonstrates that the attenuation is being handled correctly in the volume potential method. 286

The first five harmonics along the x-axis are shown in Fig. 5 and Fig. 6. In both cases we

287 V. COMPUTATION DOMAINS FOR SUCCESSIVE HARMONICS

In this section we aim to determine the amount by which we can restrict the computation domain while retaining accurate approximations, and thus enable acceleration of our simulations.

The main region of interest to practitioners is that around the focus, since this is where tissue ablation occurs. Ideally one would compute only on that small region. This, however, leads to the second harmonic (and thus also the third, fourth, etc.) being poorly approx-

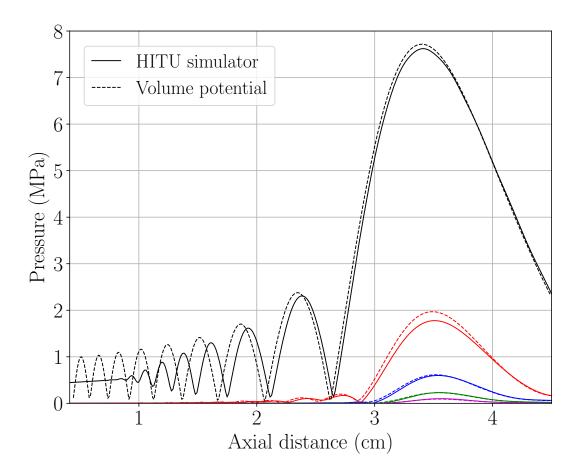


FIG. 5. Comparison of the VIE approach with HITU simulator for the first five harmonics generated by the H131 transducer operating at a power of 50W in water.

imated since these harmonics are generated by the accumulation of acoustic energy over distance. So we seek a balance between accuracy and computational cost. Here we shall aim to keep the error in each harmonic below 1% (relative to the magnitude of the first harmonic) whilst shrinking the integration regions D_i in (12)-(16) as much as possible.

It is important to note that (in this homogeneous setting), the field beyond the focal point
has no influence on the field in front of it, i.e., the waves propagate only in the positive xdirection. This means that our exploration of domain shrinking only applies to the region

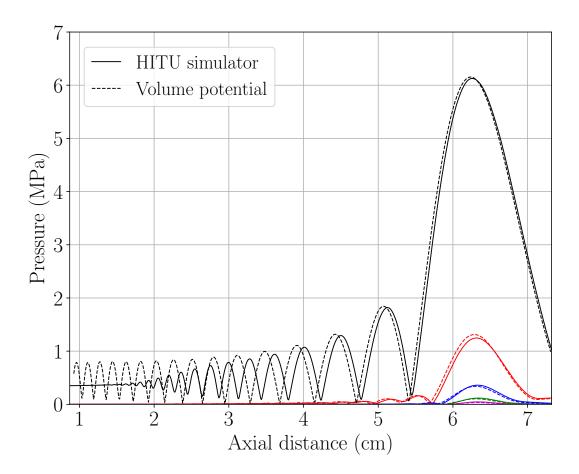


FIG. 6. Comparison of the VIE approach with HITU simulator for the first five harmonics. H101 transducer at power 100W in liver.

between the transducer and the focal point. Beyond the focus we keep the domain length in
the x-direction fixed. In most HIFU settings, the practioners are not interested in the field
far beyond the focal region, therefore the inability to shrink the region beyond the focus
does not greatly affect the gains achieved from shrinking the computational domain before
the focus.

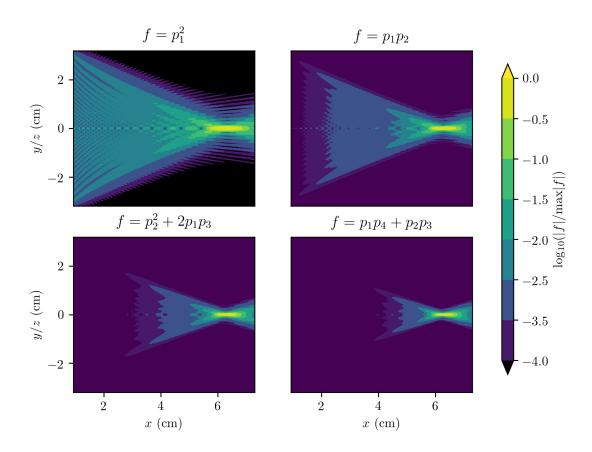


FIG. 7. The relative magnitudes of the right-hand side functions f as described in equation (24) for the H101 transducer in liver, at 100W. These plots show how the function to be convolved with the Green's function becomes more localised as the harmonics increase.

Each of the equations (12)-(16) has the form

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$$p(\mathbf{x}) = C \int_D G_k(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}, \qquad (24)$$

where $f = p_1^2, p_1 p_2, \ldots, C$ is the appropriate constant, and k is the appropriate wavenumber. In order to accurately approximate p, the integration domain D must enclose the region where the integrand is non-negligible. Outside of this region, we can discard the contribu-

of intensity. In order to have an idea of how localised the different functions f are, we 311 plot them for a particular example in Fig. 7. The setup considered in the figure is the H101 312 transducer at 100W in liver. The figure shows the magnitudes of f scaled by their maximum values (at the focus) and converted to a log-scale. Consider the top-left image: this is the 314 f required for the computation of the second harmonic. We can see that the magnitude is 315 significant all the way back to the transducer, implying that we must include all this area in the integration domain D. For the remaining images, corresponding to the third, fourth 317 and fifth harmonics, the functions become increasingly more localised in both the x and y/z318 dimensions, suggesting that the required integration domain can be considerably smaller 319 than that for the second harmonic. 320

To investigate this more rigorously, we perform convergence tests for each harmonic as
the relevant integration domain D is restricted. That is, we take the harmonics generated
on the domain in (21) as the reference solutions p_l^r , l=2,3,4,5, and then compute the
same harmonics on successively smaller domains and compare the approximations to the
reference. The error of an approximation p_l is computed along the x-axis as

Error =
$$\frac{||p_l - p_l^r||}{||p_l^r||} \times 100\%$$
. (25)

Note that the harmonic field in the denominator is that of the first harmonic. This is done so that the error function incorporates the diminishing size of successive harmonics. For example, if the fifth harmonic is negligibly small relative to the first harmonic (and so not worth calculating), the error will reflect this by being very small. As a measure of the "localisedness" of the functions f, we use the quantity plotted in Fig. 7, which we denote as Q:

$$Q(\mathbf{x}) := \log_{10} \left(\frac{|f(\mathbf{x})|}{\max|f(\mathbf{x})|} \right). \tag{26}$$

In the convergence tests, the integration domain is chosen as the smallest cuboidal domain D such $Q(\mathbf{x}) < Q_0$ for $\mathbf{x} \notin D$, where Q_0 is a given threshold.

The first configuration we test is the H131 transducer in water at an output power of 100W. The convergence for each harmonic is shown in Fig. 8. We notice that the convergence of the second harmonic drops suddenly once the error dips below 1% – this is because the computation domain is close to the size of the reference domain by this point. This is illustrated more clearly in Fig. 9 where the same data as in Fig. 8 is shown but now plotted against the size of the computation domain as a fraction of the reference domain, rather than against Q_0 . It shows that, to achieve less than 1% error in p_2 , the computation domain must extend all the way to the transducer.

For the higher harmonics, however, a different trend is evident. In Fig. 8 we observe that
the error curves for p_3, p_4, p_5 each have the approximate behaviour

$$\operatorname{Error}(p_i) \approx 10 \frac{||p_i||}{||p_1||} \sqrt{Q_0}, \quad i = 3, 4, 5,$$
 (27)

where $||\cdot||$ represents the L^2 -norm. Although an interesting observation, the utility of the relationship (27) for dictating an appropriate computation domain for p_i is not immediately apparent, since it requires the computation of $||p_i||$ before p_i has been computed. Determining an *a priori* approximation for $||p_i||$ to make use of (27) would be a useful endeavour, however we do not undertake such a task in this article. Rather we seek to develop an ap-

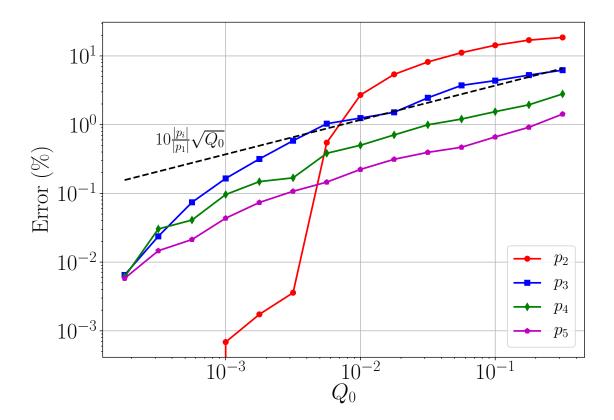


FIG. 8. Convergence of the approximations to harmonics p_i , i = 2, ..., 5 as the domain of integration D_i for each is adjusted according to the function $Q \ge Q_0$, as defined in (26). The setup considered here is the H131 transducer at a power of 100W in water.

proximate rule of thumb for choosing sensibly-sized computation domains for the harmonics.

To this end, it is more straightforward to consider the convergence of the approximations in

terms of physical distance, as is done in Fig. 9 and Tab. III.

By looking at the 1% error line in Fig. 9, it is possible to read off the size of the domains
as fractions of the reference domain. The precise values are reported in Tab. III. A nested
series of domains constructed according to this specification is shown in Fig. 10. Let us

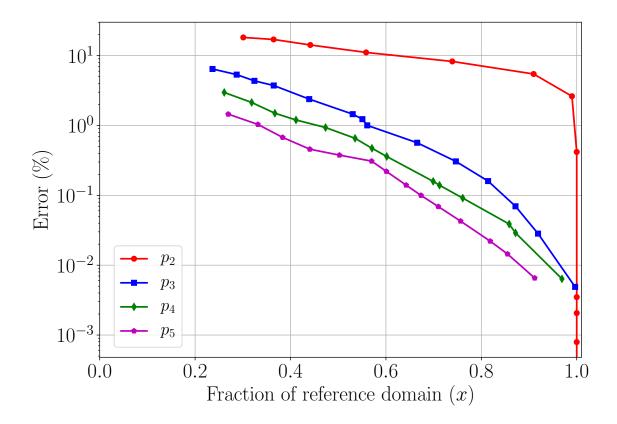


FIG. 9. Convergence for H131 transducer at 100W in water, as in Fig. 8, but now the error is plotted against the fraction of the total domain in the x-direction. This demonstrates that, to achieve an error smaller than 1%, the computation domains can be contracted significantly in the x-direction for harmonics higher than the second.

elaborate on the potential computational gain achieved using these nested domains compared to computing all harmonics on the reference domain.

The reference domain for the H131 transducer in water has dimensions [4.1cm, 3.3cm, 3.3cm] and is discretised into voxels of dimension $\delta x = \lambda_5/6 \approx 4.51 \times 10^{-5} \text{m}$, i.e., fine enough to resolve the highest harmonic of interest. This mesh has $901 \cdot 732 \cdot 732 \approx 4.8 \times 10^8$ voxels for the computation of all the harmonics. Using the nested domains built according to

the specifications in Tab. III, we obtain a mesh for p_2 with dimensions [4.1, 2.4, 2.4]cm,
which is discretised into voxels of dimension $\delta x = \lambda_2/6 \approx 1.13 \times 10^{-4}$ m. This mesh has $360 \cdot 211 \cdot 211 \approx 1.6 \times 10^7$ voxels, which is a factor of 30 smaller than the reference mesh.

The meshes for the higher harmonics have even fewer voxels and so overall we achieve more
than a factor 30 reduction in computational load compared to computing all harmonics on
the reference mesh.

		p_2	p_3	p_4	p_5
H131 water	x	1	0.67	0.47	0.38
100W	y/z	0.74	0.39	0.20	0.13
H131 water	x	1	0.67	0.58	0.52
150W	y/z	0.71	0.40	0.39	0.21
H131 liver	x	1	0.56	0.25	0.26
100W	y/z	0.90	0.20	0.05	0.06
Rule of	x	1	0.75	0.65	0.61
thumb	y/z	1	0.67	0.5	0.4

TABLE III. Sizes of domains required to achieve less than 1% error for each harmonic as fractions of the reference domain (21). Since all domains are boxes, the fractions of the distances in the x and y/z directions are provided.

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This improvement is impressive, however it is easily seen in Tab. III that this particular domain scaling does not apply to all transducer and material configurations. Therefore, we decide upon a simple rule of thumb for designing the separate computational domains that leads to domains greater than or equal to those given in Tab. III. Therefore, the errors incurred in using these domains will be even smaller than those obtained when using the ideal domains specified in the table.

A desirable rule for domain sizes would be the following:

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Let [l+d,w,w] be the dimensions of domain D_2 (see Fig. 1) for harmonic p_2 ,
with corresponding wavelength λ_2 . Then choose the dimensions of domain D_i , i>2, as $[\frac{\lambda_i}{\lambda_2}l+d,\frac{\lambda_i}{\lambda_2}w,\frac{\lambda_i}{\lambda_2}w]$. That is, the domain is scaled according to the
wavelength of the harmonic being considered.

With this rule for creating the domains, we observe that the number of voxels in each mesh will almost be the same, save for a slight increase due to the fact that the distance d is not being scaled. This amounts to a reduction in the overall number of DOF by a factor of approximately $(n/2)^3$ (in fact, slightly lower than this due to the unscaled portion of length d), where n is the number of harmonics being computed.

In the next section, we outline an algorithm for evaluating the volume potentials over a set of nested domains constructed according to the rule of thumb proposed above.

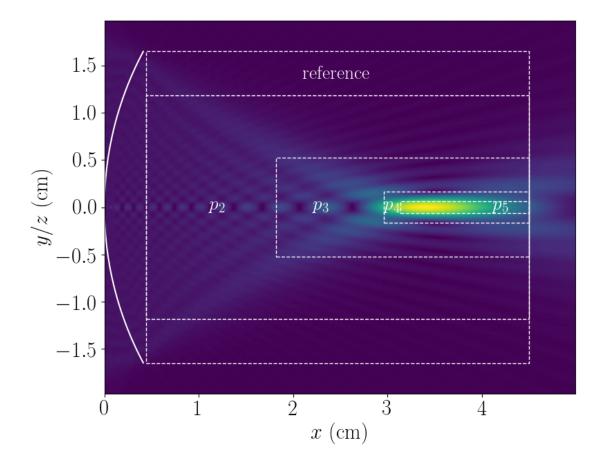


FIG. 10. Nested domains for the computation of successive harmonics while keeping relative error below 1%, for the H131 transducer operating at 100W in water. The domain used to compute the reference solution is in (21).

9 VI. VOLUME POTENTIALS ON NESTED MESHES

To demonstrate the effectiveness of the volume potential evaluation on nested meshes, we present some final results detailing the computational performance of this approach. First we outline the algorithm for computing the first n harmonics:

for $i = 2 \rightarrow n$ do

	N° voxels	Meshing	Interpolation	Evaluate G_{k_i}	Compute p_i
p_2	1.86×10^8	26.1s	24 m 30 s	4m54s	3m48s
p_3	2.01×10^{8}	22.2s	3 m 9 s	5 m 14 s	4m9s
p_4	2.15×10^8	23.9s	5 m 50 s	5 m 27 s	4m8s
p_5	2.30×10^8	25.5s	$7 \mathrm{m} 12 \mathrm{s}$	$6 \mathrm{m} 7 \mathrm{s}$	$7 \mathrm{m} 5 \mathrm{s}$

TABLE IV. Performance details for the volume potential approach on nested meshes with a resolution of six voxels per wavelength (for each harmonic). The configuration considered is the H101 transducer operating at 100W in water. Total time taken 1h23m11s.

- 1. Create domain D_i for p_i and voxel mesh $\mathcal{V}(D_i)$
- 2. Assemble components for integration (17):
- (a) Evaluate/interpolate $p_{i-1}, p_{i-2}, \dots, p_1$ at voxel centres in $\mathcal{V}(D_i)$
- (b) Evaluate integral of Green's function G_{k_i} over each voxel
 - 3. Compute p_i via appropriate equation in (12)–(16)

end for

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Note that in the above algorithm, for p_2 , the pressure field p_1 is evaluated over the voxel mesh $\mathcal{V}(D_2)$ as described in Section IIIB. Whereas for later harmonics we perform interpolation of the earlier harmonics down onto the new mesh. In this work we have used linear interpolation, however if higher accuracy is required, we recommend quadratic interpolation (albeit at a higher computational cost). The second and third step each contain applications of the FFT: for the circulant embedding of the Green's function in step 2 (see, e.g., (Groth

et al., 2020)) and to perform the convolution required in the quadrature rule (17) in step 3.

These FFTs are performed using the Python wrapper 'pyfftw' to the FFTW library (Frigo and Johnson, 2005).

As an example, we consider the H101 transducer operating at 100W in water run on a workstation with two sockets, each containing a 14-core Xeon E5-2690 v4 CPU, each supporting hyper-threading with two threads, and hence a total number of 56 threads. The total amount of RAM available on this machine is approximately 270GB, which is ample for the problems considered here. The first five harmonics along the x-axis are shown in Fig. 11, along with the approximation obtained with HITU simulator; again we see that the volume potential approach predicts a larger peak in the second harmonic but in general a good qualitative agreement is observed.

To get a feel for the performance of our approach (of evaluating the volume potentials 417 on nested meshes designed according to our proposed rule of thumb), the cost of each step 418 in the above algorithm is detailed in Tab. IV. The largest mesh has 230 million voxels, as 419 compared to 2.9 billion voxels without nested meshing. This represents a large saving, in both time and memory. The most expensive step reported in Tab. IV is the evaluation 421 of the first harmonic p_1 on $\mathcal{V}(D_2)$. This process was described in Section IIIB and has 422 complexity $\mathcal{O}(n_e N)$, where n_e is number of points used to discretise the surface of the transducer and N is the number of voxels. Since we take $n_e = 4096$, this is a rather 424 expensive procedure, even when parallelised over 56 threads. Therefore a transducer model 425 using far fewer elements and/or a machine with more threads will lead to a large reduction 426 in computation time for this step. Linear interpolation is computed efficiently using the scipy (Jones et al., 2001–) RegularGridInterpolator command. The evaluation of G_{k_i} consists of a parallelised loop over the N voxels and then an FFT of a three-dimensional complex-valued array of size $(2N_x, 2N_y, 2N_z)$, where N_x, N_y, N_z are the number of voxels in each dimension. Then the computation of p_i consists of one forward and one inverse FFT of an array of size $(2N_x, 2N_y, 2N_z)$. The FFTs take advantage of multithreading, therefore can be easily accelerated through the use of more cores. Furthermore, it seems likely that optimising the FFT routine for the particular setting and using the FFTW C++ library directly will lead to further acceleration. Nevertheless, the current implementation yields fast and accurate predictions of the first five harmonics (in the cases considered).

437 VII. CONCLUSION

In this paper we have set out to reduce the computational burden of numerical schemes for HIFU simulations through the construction of an efficient and simple meshing strategy.

This strategy can be employed with those numerical schemes that allow for non-uniform meshes, such as finite element methods, and those that solve for each harmonic on separate meshes, such as the frequency-domain volume potential approach proposed here.

The strategy exploits the increasingly localised nature of the higher harmonics around the transducer's focal region so that the degrees of freedom in the mesh can be more efficiently distributed. If we were considering a single mesh in a finite element approach, for example, this mesh would become increasingly more refined toward the focus, since this is where the higher harmonics are present. In the frequency-domain setting, this leads to a nested series of meshes, as was discussed in detail in this article.

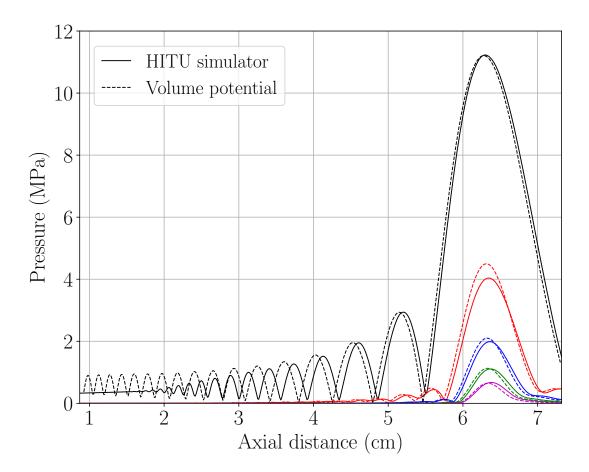


FIG. 11. The on-axis absolute pressure field for the first five harmonics generated by the H101 transducer at 100W in water, as computed using the volume potential approach on nested domains, designed to keep the relative error below 1%. The approximation obtained using the HITU simulator is provided for comparison.

In the frequency domain, the Westervelt equation can be rewritten as a series of inhomogeneous Helmholtz equations. When the propagation medium is taken to be homogeneous, these Helmholtz equations can be solved exactly by volume potentials, which may be efficiently evaluated using the quadrature method proposed in Section III. This novel application of this approach allow us to explore efficiently the convergence of each harmonic

as the respective computation domain was changed in size. Thus enabling us to determine
the smallest domains we could use in order to achieve an error of less than 1%.

We showed that the accurate approximation of the second harmonic requires a computation domain that extends from the focus all the way to the transducer, since the first 457 harmonic is not sufficiently localised near the focus to allow a smaller domain to be employed. 458 The third harmonic and above, however, can be approximated accurately on considerably reduced domains. We found that scaling the computation domain's width and height rela-460 tive to the wavelength under consideration allowed for accurate approximations for the first 461 five harmonics for the HIFU configurations considered here. This leads to a reduction in the 462 number of degrees of freedom of approximately $(n/2)^3$, where n is the number of harmonics 463 being computed. 464

In addition to being of use to finite element methods, the volume potential approach could
be extended to inhomogeneous/scattering configurations by the introduction of boundary
and volume integral operators. Such an extension is left to future work.

A Python implementation of this work is freely available at github.com/samuelpgroth/vines.

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