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# Scattering Evaluation of Equivalent Surface Impedances of Acoustic Metamaterials in Large FDTD Volumes Using RLC Circuit Modelling

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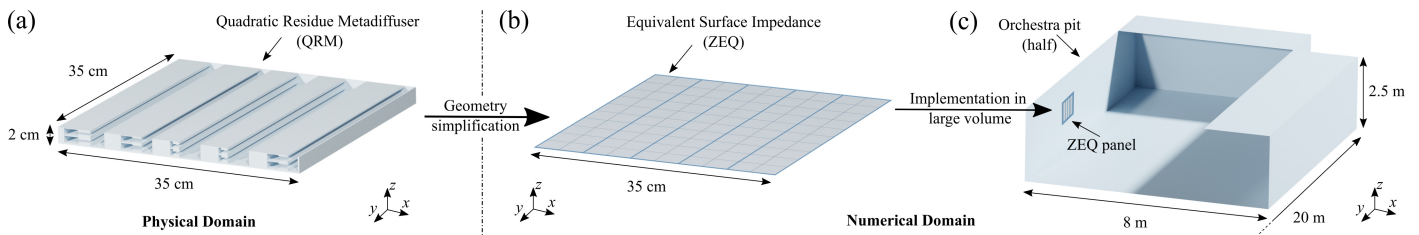
**Abstract:** The majority of simulations involving metamaterials often require complex physics to be solved through refined meshing grids. However, it can prove challenging to simulate the effect of local physical conditions created by said metamaterials into much wider computing sceneries due to the increased meshing load. We thus present in this work a framework for simulating complex structures with detailed geometries, such as metamaterials, into large Finite Difference Time-Domain (FDTD) computing environments by reducing them to their equivalent surface impedance represented by a parallel-series RLC circuit. This reduction helps to simplify the physics involved as well as drastically reducing the meshing load of the model and the implicit calculation time. Here, an emphasis is made on scattering comparisons between an acoustic metamaterial and its equivalent surface impedance through analytical and numerical methods. Additionally, the problem of fitting RLC parameters to complex impedance data obtained from transfer matrix models is herein solved using a novel approach based on zero crossings of admittance phase derivatives. Despite the simplification process, the proposed framework achieves good overall results with respect to the original acoustic scatterer whilst ensuring relatively short simulation times over a vast range of frequencies.

**Keywords:** Metamaterials; metadiffusers; scattering; finite-difference time-domain (FDTD)

## Introduction

Over the past decades, there has been a lot of progress regarding numerical simulation techniques in the field of wave physics, mostly benefiting from modern hardware and software improvements. Yet, computing limits can still be reached in most frequency- or time-domain numerical problems. Both approaches come with their own strategies for approximating wave equations within a bounded space. Usually, the accuracy and computational time of such schemes are dependent on the minimal size of the meshing grid, on the hardware at hand, the frequency to be studied, and on the overall size of the numerical environment. To a relative degree, numerical schemes tend to be computationally cheaper for modelling either complex geometries in small spaces or simpler geometries within larger spaces. The suitability of one method over the other generally depends on the scope of the study.

There are cases, however, where simulations of complex geometries in larger sceneries are of specific interest, i.e., sceneries where intricate geometry with fine meshing is required at a local scale, but the physical effect of such geometry has to be studied within a much more global environment. An example of such study can be found in simulations involving metamaterials, which are usually quite compact, where their influence over a larger three-dimensional context may be of interest. Metamaterials are composite structures engineered in such way that they can display extraordinary physical properties within deep-subwavelength dimensions, i.e., dimensions much smaller than the design



**Figure 1.** Conceptual diagram illustrating (a) a render of a Quadratic Residue Metadiffuser (QRM) with  $N = 5$  slits, (b) a numerical equivalent surface impedance (ZEQ) of the metadiffuser identically composed of  $N = 5$  slits, and (c) an implementation of the ZEQ into a large computational volume, e.g., an orchestra pit.

37 wavelength. As such, metamaterials come in a variety of shapes for many wave control  
 38 applications, going from frequency selective structures for cloaking [1] or trapping [2] to  
 39 reconfigurable radiation patterns for imaging [3] and telecommunications [4], with scales  
 40 ranging from optical [5] to seismic [6] wavelengths, passing through microwave [7],  
 41 ultrasound [8] and audio frequencies [9]. In the case where the volume of the simulated  
 42 scenery happens to be very large compared to the metamaterial meshing dimensions,  
 43 traditional modelling strategies could prove non-viable within realistic means; likely  
 44 resulting in immense computational times and memory requirements. This calls for alter-  
 45 native strategies in modelling local wave interactions at boundaries and their respective  
 46 propagation behaviour in much larger spaces within more reasonable computational  
 47 means.

48 This problematic has sprung a rising number of research initiatives for many  
 49 decades. The concept of impedance [10] has helped in establishing a strategy for ap-  
 50 proximating the physical conditions created by the geometry of an object by a set of  
 51 impedance boundary conditions (IBC) [11]. Many of such investigations began to appear  
 52 in numerical applications linked to electro-magnetic [12,13], heating [14], and acous-  
 53 tic [15] problems in order to reduce the computational load; particularly so in the early  
 54 years of scientific computer simulations. Lately, this strategy has seen multiple uses for  
 55 simplifying intricate subwavelength structures, such as metamaterials [16–19]. On top  
 56 of analytical impedance approximations, the Resistor-Inductor-Capacitor (RLC) circuit  
 57 impedance analogy between electrical and mechanical systems [10] has also allowed  
 58 for simpler expressions of resonant structures. This becomes notably useful for the  
 59 description of metamaterials made of locally-resonant elements [20]. In the context of  
 60 large scale acoustic computation, time-domain methods offer the advantage to simulate  
 61 a vast range of frequencies for large spaces in a single computation run [21]. Many of  
 62 the works in this field emphasize on the use of frequency-dependent boundary condi-  
 63 tions as a means to describe the acoustic characteristics of the interfaces present in the  
 64 model [22–29]. However, to the authors knowledge, no work has yet been conducted  
 65 for applying metamaterial-based impedance boundary conditions into large-scale time-  
 66 domain acoustic computational methods.

67 In this work, we propose an acoustic scattering study where compact metamaterial-  
 68 inspired acoustic diffusers, called *metadiffusers* [30–32], are considered too complex to  
 69 simulate directly in a 3D finite-difference time-domain (FDTD) scheme, and thus decide  
 70 to evaluate the computational and scattering impact of RLC IBCs on the diffuse field  
 71 of a larger space in which they could be installed, such as an orchestra pit. Figure 1  
 72 illustrates this approach, where the scaled scheme of a  $N = 5$  slits Quadratic Residue  
 73 Metadiffuser (QRM) used here as a reference compact metamaterial is shown in Fig.  
 74 1(a). The local scattering generated by the metadiffuser can be alternatively reproduced  
 75 through a simplification of the metamaterial geometry into a set of IBCs. The resulting  
 76 IBCs can thereafter be reproduced through an RLC circuit [28] integrated at the desired  
 77 boundaries of the 3D FDTD volume, as illustrated in Figs. 1(b,c). The novelty of this  
 78 approach lies in the optimized fitting of the RLC circuit IBCs based on zero crossings of  
 79 admittance phase derivatives in order to ultimately replicate the scattering generated

80 by metamaterial structures in large FDTD volumes. A time-domain scheme has been  
 81 chosen for this work as not only it can wield broadband frequency information, but also  
 82 enables time-domain signal processing which can later be used for further virtual audio  
 83 operations for auralization and spatialization purposes.

## 84 1. Theoretical Modelling

85 Acoustic scattering occurs when a travelling sound wave encounters an obstacle or  
 86 inhomogeneity in its path, e.g., a solid object or a change of medium density, and thus  
 87 breaks into secondary spreads out from it in a variety of directions. The magnitudes  
 88 and directions of such scattered waves can be described by the Helmholtz-Kirchhoff's  
 89 theory of diffraction, which uses Green's theorem to determine the scattered pressure  
 90 at any given point by specifying the wave field onto the scattering obstacle. However,  
 91 the latter formulation is generally approximated depending of contextual assumptions  
 92 regarding the distance of the source and observer from the scattering object compared to  
 93 the monochromatic wavelength. This leads to two major situations, i.e., (i) the near-field  
 94 where the source and observer are relatively close to the obstacle, under the Rayleigh  
 95 critical distance ( $R_0 = S/\lambda$ , where  $S$  is the area of the surface and  $\lambda$  the wavelength of  
 96 the wave), and (ii) the far-field where the source and observer are considered to be far  
 97 away from the obstacle, in the limit of infinity.

On a first instance, we will focus on the frequency dependent scattering made by  
 the metasurface, where the acoustic field at a point  $\mathbf{r} = \mathbf{r}(x, y, z)$  scattered by a surface  
 centred at  $\mathbf{r}_0 = \mathbf{r}(x, y, z = 0)$  can be approximated by the Rayleigh-Sommerfeld integral  
 as

$$P_s(\mathbf{r}) = -i \frac{k}{2\pi} \int_{S_0} \frac{p_0(\mathbf{r}_0)R(\mathbf{r}_0)e^{jk|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|} dS, \quad (1)$$

where  $p_0(\mathbf{r}_0)$  is the incident pressure field, and  $R(\mathbf{r}_0)$  is the spatially dependent reflection  
 coefficient of the locally reacting surface  $S_0$ , with  $k = \omega/c_0$  being the wavenumber  
 in air at the angular frequency  $\omega$  and speed of sound  $c_0$ . Here, the Fourier transform  
 of  $f(x)$  is  $\hat{f}(k)$ , which is given by  $\hat{f}(k) = \int f(x)e^{-jkx}dx$ . It transpires from Eq.(1) that  
 defining the state of the spatially dependent reflection coefficient,  $R(\mathbf{r}_0)$ , is ultimately  
 important in order to determine the directions and magnitudes of the scattered sound  
 energy. In the case of metadiffusers, the spatially-dependent surface reflection coefficient  
 is obtained through the Transfer Matrix Method [30] (TMM), which relates the acoustic  
 pressures and normal particle velocities at the extremities of a one-dimensional acoustic  
 system; here, a slit loaded with Helmholtz resonators (HRs). The surface reflection  
 coefficient and characteristic impedance of the  $n$ -th slit,  $R_{slit}^n$  and  $Z_{slit}^n$ , respectively, can  
 be interchangeably deduced one from the other by the relation

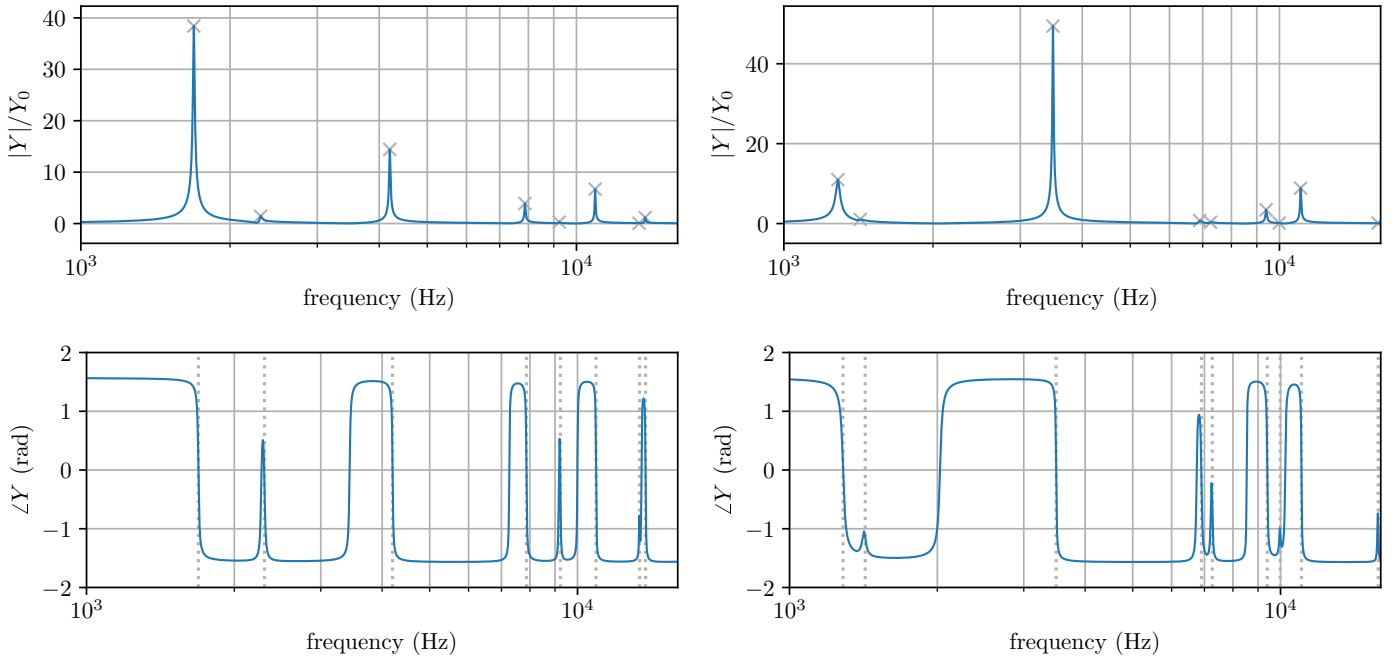
$$Z_{slit}^n = Z_0 \frac{1 + R_{slit}^n}{1 - R_{slit}^n}, \quad (2)$$

98 where  $Z_0 = \rho_0 c_0$  is the characteristic impedance of air.

The diffusion coefficient of a surface rates the uniformity of the aforementioned scat-  
 tered sound field. Moving to a spherical coordinate system where  $P_s(\mathbf{r}) = P_s(\theta, \phi, r)$  with  
 $\theta$  and  $\phi$  being the elevational and azimuthal planes respectively and  $r$  being the distance  
 to the origin, the directional diffusion coefficient[33],  $\delta_\psi$ , produced when a sound dif-  
 fuser is radiated by a plane wave at the incident angle  $\psi = (\theta', \phi')$  (primed superscripts  
 denoting incident angles), can be estimated from the hemispherical autocorrelation of  
 the scattered distribution

$$\delta_\psi = \frac{\left[ \iint I_s(\theta, \phi) dS \right]^2 - \iint I_s^2(\theta, \phi) dS}{\iint I_s^2(\theta, \phi) dS}, \quad (3)$$





**Figure 2.** Normalized magnitude and phase of two example surface admittances (left and right) of two different slits within a QRM as a function of frequency in Hz, with identified resonances marked in grey dots.  $Y_0 = 1/\rho_0 c_0$  represents the admittance of air.

99 where  $I_s(\theta, \phi) \propto |p_s(\theta, \phi)|^2$  is proportional to the scattered intensity. The integration is  
 100 performed over a hemispherical surface ( $-\pi/2 \leq \theta \leq \pi/2$  and  $0 < \phi < 2\pi$ ) where  
 101  $dS = d\theta d\phi$ . This coefficient must be normalized to that of a plane reflector,  $\delta_{flat}$ ,  
 102 so as to eliminate the diffracting effect caused by the finite size of the structure, i.e.,  
 103  $\delta_{n,\psi} = (\delta_\psi - \delta_{flat}) / (1 - \delta_{flat})$ . In this work we analyse the 3D case of a normal incident  
 104 wave, i.e.,  $(\theta', \phi') = (0, 0)$  and  $\delta_{n,\psi} \equiv \delta_{n,0}$ .

## 105 2. RLC Circuit Impedance Boundary Formulation

106 The magnitude and phase of the surface impedance of a metadiffuser are marked  
 107 by the inherent resonances of the structure, i.e., if it has one or more resonators it should  
 108 show one or more fundamental resonant peaks or phase shifts in its surface impedance.  
 109 In the case of the QRM, a highly resonant structure with two HRs per slit is displayed,  
 110 which lends itself to a boundary formulation based on a combination of second-order  
 111 resonators. Example admittances for two slits of the QRM are shown in Fig. 2. The two  
 112 slits displayed in Fig. 2 are both loaded with two HRs but with different slit and HR  
 113 dimensions. This results in different surface impedances for each slit, thus presenting  
 114 different resonance peak amplitudes and phase-shifts.

One useful passive formulation for a given slit impedance consists of a parallel set  
 of series-RLC circuits (after [28]), each consisting of one resistor (R), one inductor (L)  
 and one capacitor (C), where all RLC parameters are non-negative and real-valued. The  
 admittance of this structure in the Laplace domain is given by

$$Y(s) = \sum_{b=1}^B \frac{1}{Z^{(b)}}, \quad Z^{(b)} = L^{(b)}s + R^{(b)} + 1/(sC^{(b)}), \quad (4)$$

115 where  $L^{(b)}$ ,  $R^{(b)}$ , and  $C^{(b)}$  are non-negative constants for each branch. For our analyses  
 116 and optimizations, we can limit  $s$  to  $s = j\omega$ , and where  $B \geq 1$  is the number of RLC  
 117 branches. The associated impedance of the RLC circuit is then simply  $Z(j\omega) = 1/Y(j\omega)$ .  
 118 With this impedance boundary formulation we aim to fit the surface impedance of each  
 119 slit of the QRM with an equivalent circuit made up of a set of resonances with non-negative

120 RLC parameters. The passivity of this structure is then preserved in the discrete FDTD  
 121 setting through the choice of the bilinear transform as a discretisation method [34]. This  
 122 impedance model can be seen as an extension of various simpler frequency-dependent  
 123 boundary models presented in the context of FDTD methods for room acoustics [35–37].

124 A methodology for fitting RLC parameters is described in [28], which consists of:  
 125 (i) identifying resonances in an admittance by their peaks in the admittance magnitude,  
 126 and (ii) estimating half-power bandwidths for each resonance from admittance magni-  
 127 tude. From those estimates RLC parameters may be identified for each resonance. This is  
 128 followed by a global optimization over the RLC triplet parameters using a Nelder-Mead  
 129 optimization. That approach works well when admittance peaks are well-separated,  
 130 but in general peaks in admittance magnitude data can be difficult to identify, and  
 131 furthermore half-power bandwidths can be hard to estimate from admittance magnitude  
 132 data alone. This is especially true in the example admittances shown in Fig. 2. Other  
 133 ways for approximating the weight and resonant frequencies in viscoacoustic problems  
 134 were also previously reported [38].

In this study we use an approach which is based on making use of admittance  
*phase* information, and derivatives thereof, to identify resonance parameters. It can be  
 observed from Fig. 2 that peaks in admittance magnitude are linked to inversions in the  
 phase response. More specifically, we know that the phase response of an individual  
 series-RLC circuit admittance goes to zero at its resonant frequency and also displays a  
 negative slope at that frequency. Additionally, regarding the slope of the phase at the  
 resonant frequency, one can derive from Eq. 4

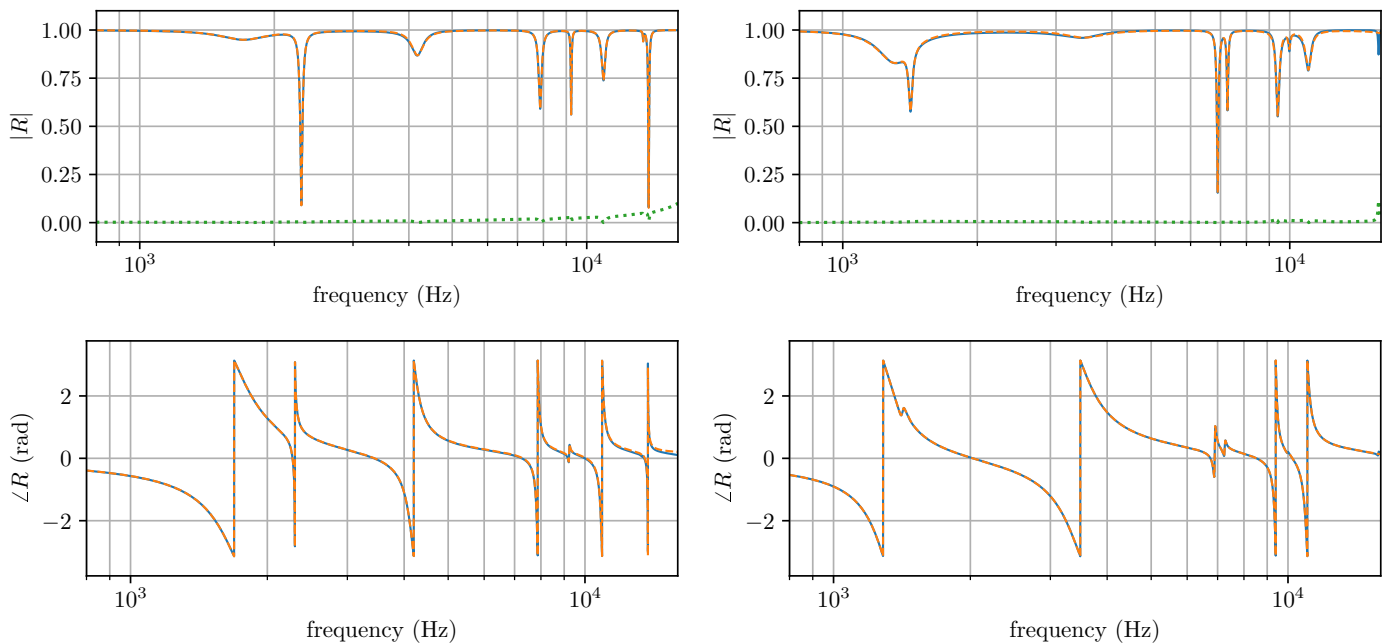
$$-\left. \frac{\partial \angle Y(j\omega)}{\partial \omega} \right|_{\omega=\omega_0} = \frac{2}{\Delta\omega} = \frac{2L}{R}, \quad (5)$$

where  $\omega_0 = 1/\sqrt{LC}$ . Thus, after detecting a resonance in the admittance phase from  
 its slope and zero crossings, and after sampling the associated peak in the admittance  
 magnitude, the half-power bandwidth,  $\Delta\omega$ , follows from Eq. (5) (which may be estimated  
 with simple finite differences). This approach is sufficient to obtain RLC parameters  
 for each well-isolated resonance, and can be more robust than peak detection and half-  
 power bandwidth estimation from the admittance magnitude alone. Nevertheless, this  
 approach still has limitations for very-closely spaced resonances (examples can be seen  
 in Fig. 2) where the phase response at a resonance may not cross zero (and thus would  
 not be detected with this approach so far). To deal with such issues, the *second derivative* of  
 the phase is additionally used to identify resonances, which can be written as:

$$\left. \frac{\partial^2 \angle Y(j\omega)}{\partial \omega^2} \right|_{\omega=\omega'_0} = 0, \quad \omega'_0 = \omega_0 \sqrt{\sqrt{4 - (\Delta\omega/\omega_0)^2} - 1}, \quad (6)$$

135 where  $\omega'_0$  is the angular frequency at which there is a zero crossing in the second-order  
 136 derivative of the admittance phase. Furthermore  $\omega'_0 \approx \omega_0$  provided that  $(\Delta\omega/\omega_0)^2 \ll 1$ ,  
 137 which means that  $\omega'_0$  may be used as an initial estimate of  $\omega_0$  to seed the subsequent  
 138 global optimisation. Identified resonances using this phase-derivative zero-crossing  
 139 method (grey dotted lines) can be seen in Fig. 2.

140  
 141 Once a set of RLC triplet parameters has been identified given a set of resonant  
 142 frequencies and associated bandwidths, a global optimization using a Nelder-Mead  
 143 method [39] as a non-linear minimization algorithm is carried out to find the  $L^{(b)}$ ,  $R^{(b)}$   
 144 and  $C^{(b)}$  that minimize  $\epsilon = \|Y_{TMM} - Y_{RLC}\|$ , where, for a given slit,  $Y_{TMM}$  is the target  
 145 admittance output from the TMM model of the QRM, and  $Y_{RLC}$  is the impedance output  
 146 of the RLC circuit. Fit reflection coefficients of the two QRM slits previously illustrated  
 147 (see Fig. 2) can be seen in Fig. 3. It can be observed that this methodology is successful  
 148 in capturing the resonances within the QRM slits. The errors shown take into account  
 149 magnitude and phase, and discrepancies can be seen at the upper limit of our range of



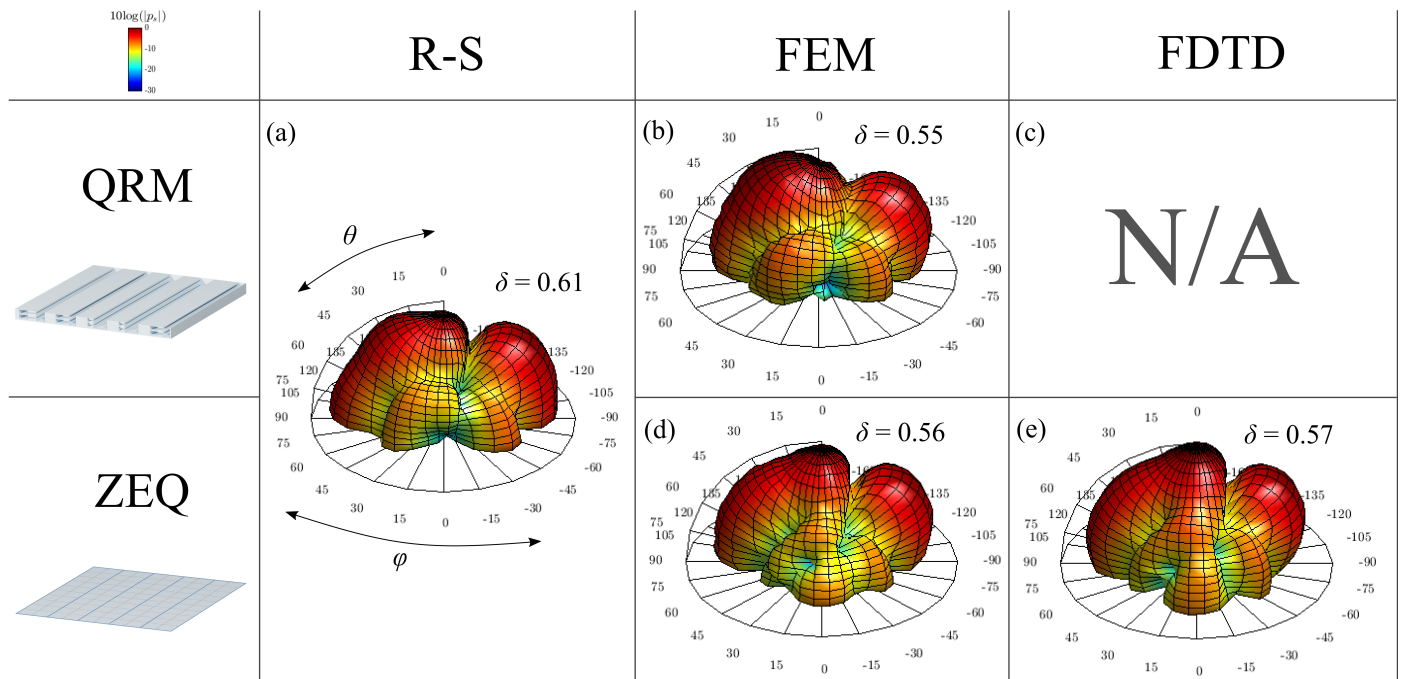
**Figure 3.** Magnitude and phase of the reflection coefficient using the Transfer Matrix Method (blue, solid) and using the RLC approximation (orange, dashed) relating two different slit admittances within the QRM along with fitting errors (green, dotted), as a function of frequency in Hz.

150 frequencies (e.g., a resonance being ignored). Such discrepancies may be attributed to  
 151 viscothermal losses in the TMM model which cause deviations from ideal second-order  
 152 resonances. These could be mitigated by using pairs of RLC triplets for each identified  
 153 resonance to allow for better optimised results, but this was not pursued as a compromise  
 154 of accuracy and model complexity.

155 For later comparison purposes, a similar approach for modelling the equivalent  
 156 surface impedance of the QRM is adopted in a Finite Element Method (FEM) study in  
 157 COMSOL Multiphysics 5.3<sup>TM</sup>, where the  $N = 5$  impedance patches were modelled using  
 158 built-in impedance boundary conditions with the complex impedance data obtained  
 159 from the TMM model as input. The resulting scattering data between the QRM and the  
 160 equivalent surface made of different RLC circuits is shown in the next section.

### 161 3. Spatial Acoustic Scattering

162 Figure 4 compares the 3D hemispherical scattered sound pressures of the aforemen-  
 163 tioned QRM with  $N = 5$  slits and the equivalent RLC surface impedance,  $Z_{EQ}$ , with  
 164  $N = 5$  slits as well. The scattering distributions have been obtained through different  
 165 methods, i.e., (i) the Rayleigh-Sommerfeld (R-S) integral for near-field scattering in-  
 166 formation, (ii) Finite Element Method (FEM) in COMSOL Multiphysics 5.3<sup>TM</sup>, and (iii)  
 167 Finite-Difference Time-Domain (FDTD) simulations. Numerical simulations in COMSOL  
 168 were computed by installing the surface at the centre of a spherical domain filled with  
 169 air, surrounded by a concentric perfectly matched layer (PML) with a far-field boundary  
 170 condition at the boundary of the air domain to satisfy Sommerfeld's radiation condition.  
 171 A similar setup was used in the FDTD domain, but with first-order Engquist-Majda [40]  
 172 absorbing boundary conditions at the boundary of a cubic air domain large enough to  
 173 ignore any erroneous reflections in the obtained responses. The FDTD simulation was  
 174 calibrated to have less than 1% numerical dispersion error up to 8 kHz with 10.5 points  
 175 per wavelength (PPW) using the usual Courant-Friedrichs-Lewy (CFL) condition for the  
 176 simplest 3D Cartesian scheme ( $CFL = 1/\sqrt{3}$ ), for which stability is ensured [21,41]. The  
 177 time step,  $T_s$ , considered in the simulations can be deduced from the CFL condition as  
 178  $T_s = X_s \times CFL/c$ , where  $X_s$  the spatial sampling and  $c = 343$  m/s is the speed of sound



**Figure 4.** Distribution of sound scattered pressure levels at 2 kHz for a Quadratic Residue Metadiffuser (QRM) and the equivalent surface impedance RLC circuit (ZEQ) according to Rayleigh-Sommerfeld (R-S) integral, Finite Element Method (FEM), and Finite-Difference Time-Domain (FDTD).  $\delta$  insets represent the diffusion coefficient of the scattered distributions.

179 in air. Figure 4 shows the theoretical and numerical solutions of the surface scattered  
 180 sound energy integrated over a radius distance of 1 m, so that all datasets represent a  
 181 finite framework. In the FDTD model, virtual microphones were positioned at 1 m  
 182 around the surface, which considering its edge dimensions  $(x,y)[35\text{ cm}, 35\text{ cm}]$ , should  
 183 be sufficient to depict correctly the scattered field at a frequency  $f = 2\text{ kHz}$ . FEM results  
 184 were obtained following a similar approach where the integration was performed over a  
 185 spherical near-to-far-field boundary condition of 1 m radius.

186 Overall, the polar plots displayed in Figs. 4(a,b) show some variations between  
 187 the theory and FEM simulations, with normalized diffusion coefficient values varying  
 188 from  $\delta_{n,0} = 0.61$  to  $\delta_{n,0} = 0.55$ . These can be explained through the divergence of  
 189 theoretical assumptions with respect to a numerical solving of the wave equation. More  
 190 specifically, in a theoretical framework, the surface impedance is considered locally  
 191 homogeneous for each slit, a fact that may not be entirely true in numerical terms due to  
 192 the potential evanescent coupling between slits; a phenomenon not taken into account  
 193 in the theory. As the scattered sound field is highly dependent on the distribution of  
 194 the surface's reflection coefficient, slight variations in the polar distributions can thus  
 195 be expected. Nonetheless, it can be seen that the global shapes of the QRM sound  
 196 scattering distributions are sensibly similar one to another, which can be confirmed  
 197 by their close autocorrelation values. In addition, Fig. 4(b) represents quite well the  
 198 expected main dip that defines the Quadratic Residue sequence at  $\theta \approx -20^\circ$  in the  
 199  $\phi = [-90^\circ : 90^\circ]$  elevation axis. The main axial and lateral energy lobes are also quite  
 200 well represented. However, a slightly higher energy lobe can be discerned at  $\theta = 20^\circ$   
 201 in the FEM case. This is likely due to the finite size of the surface sample in the simulation,  
 202 resulting in a decrease of the scattered sound energy at grazing angles, thus further  
 203 relatively enhancing the remaining scattered energy and slightly reducing the intrinsic  
 204 autocorrelation value. Despite such differences, the FEM model can be estimated to be  
 205 in good agreement with the theoretical prediction.

206 The missing scattering distribution under Fig. 4(c) is at the core of this work's  
 207 rationale, as it would be an unnecessarily complex task to simulate the fine features of

208 the metadiffuser in a large 3D volume . The complex physics and the small geometry  
 209 of the QRM not only would require an extremely fine meshing grid, and thus a very  
 210 high computational load for conducting the same simulations, but viscothermal losses  
 211 would have to be taken into account as well. This is why the aforementioned equivalent  
 212 surface impedance as a fitted RLC circuit within an FDTD model is proposed as a way to  
 213 bypass the numerical limitations of large scale multi-physics simulations, while faithfully  
 214 reproducing the intended scattering of the metadiffuser embedded in a larger scene. It  
 215 is worth noting that viscothermal losses inside the metasurface are implicitly encoded  
 216 by the RLC approach in the FDTD scheme. Yet, in order to strengthen the forthcoming  
 217 analysis between FEM and FDTD, scattering comparisons of a flat surface and a much  
 218 simpler acoustic diffuser (e.g., a Quadratic Residue Diffuser) can be found in the Supple-  
 219 mentary Materials, where excellent agreement between the different numerical methods  
 220 can be observed.

221 Figure 4(d) shows the scattering distribution of the equivalent surface impedance  
 222 simulated through FEM where the  $N = 5$  impedance patches were modelled using  
 223 impedance boundary conditions with input values identical to the analytical (TMM)  
 224 surface impedance of the QRM. Again, it can be observed that the main dip at  $\theta \approx -20^\circ$   
 225 is correctly reproduced, and that the main axial lobes are also in good agreement with  
 226 the theory, leading to a normalized diffusion coefficient  $\delta_{n,0} = 0.56$  close to that of Fig.  
 227 4(b). The major changes that can be distinguished compared to the FEM simulation of  
 228 the QRM are the energy distribution of the lateral lobes and the smoothing of the  $\theta \approx 20^\circ$   
 229 energy lobe. The former seems to resemble that of a flat panel scattering. Perhaps this is  
 230 due to the disappearance of the slit cavities within each impedance patch which may  
 231 cause variations from the estimated slit impedance values as these are dependent on the  
 232 free air radiation correction of the slits. More investigation on that matter is needed.

233 Figure 4(e) similarly represents the scattered sound distribution of the ZEQ in the  
 234 FDTD solver. Results are in excellent agreement with the ZEQ FEM data, with a very  
 235 similar normalized diffusion coefficient  $\delta_{n,0} = 0.57$ . A minor increase in scattered sound  
 236 energy can however be perceived between FEM and FDTD ZEQ models which also  
 237 appears in other cross-numerical comparisons that were conducted for traditional sound  
 238 diffusers and flat surfaces (see Supplementary Material). This slight energy increase in  
 239 FDTD RLC modelling may then be attributed to energy propagation modelling in each  
 240 numerical environment (FEM/FDTD), but remains nonetheless almost negligible with a  
 241 difference in diffusion coefficient of 1%.

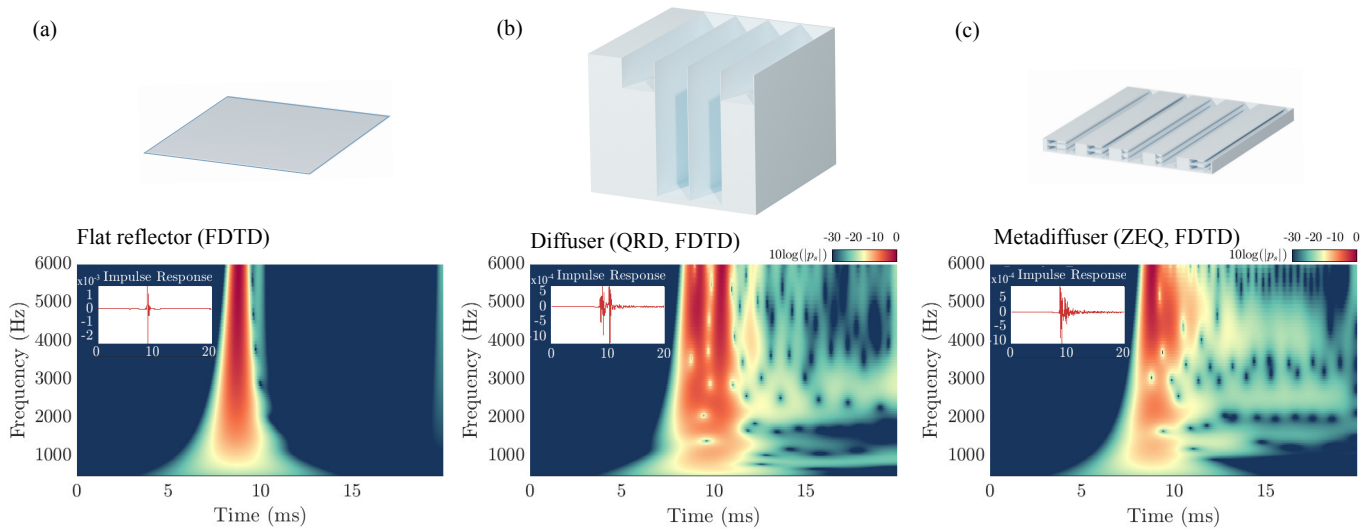
242 Whilst the equivalent surface impedance method proposed here results in a major  
 243 simplification of the more intricate geometry of the metamaterial being studied, it can be  
 244 seen that it is quite efficient for replicating an approximation of its scattered field into  
 245 the surrounding space. Also, it has been previously shown that these FDTD simulations  
 246 with such RLC circuit boundary conditions are amenable to parallel acceleration [29].

#### 247 4. Temporal Acoustic Scattering

248 In addition to the previous spatial scattering results, a temporal acoustic scattering  
 249 comparison is also here presented for evaluating the presence of time dispersion within  
 250 the above-collected FDTD data. Figure 5 thus shows several wavelet transforms of  
 251 scattered impulse responses corresponding to a flat panel, a traditional sound diffuser  
 252 and the ZEQ. A fully modelled  $N = 5$  Quadratic Residue Diffuser (QRD) of dimensions  
 253  $[x,y,z](35,35,28)$  cm and design frequency  $f_0 = 500$  Hz is here presented instead of a  
 254 QRM due to the difficulty in modelling the latter structure in the FDTD solver. One  
 255 has to note that the QRM and QRD possess different scattering characteristics over the  
 256 frequency range considered, only matching around 2 kHz.

257  
 258 Figure 5(a) shows the time-frequency information of the scattered impulse response  
 259 captured at the top of a flat surface, at  $z = 1$  m. As expected, only a single hard  
 260 reflection is obtained in the impulse response, covering the entirety of the frequency





**Figure 5.** Wavelet transforms of scattered impulse responses corresponding to (a) a flat panel via 3D FDTD, (b) the QRD via 3D PSTD, and (c) the ZEQ via 3D FDTD. Insets represent the reconstructed inverse wavelet transform of the original impulse responses.

261 range of interest. A secondary reflection with much less intensity can also be identified,  
 262 generated from the edge diffraction of the panel coming back to the receiver a couple of  
 263 milliseconds after the first major reflection. This is supported by the inset displaying  
 264 the time series of the reconstructed signal by inverse wavelet transform. Additionally,  
 265 a late reflection with small amplitude can be observed at the end of the time window  
 266 which may be due to spurious reflections not entirely absorbed by the surrounding  
 267 Engquist-Majda absorbing boundary conditions.

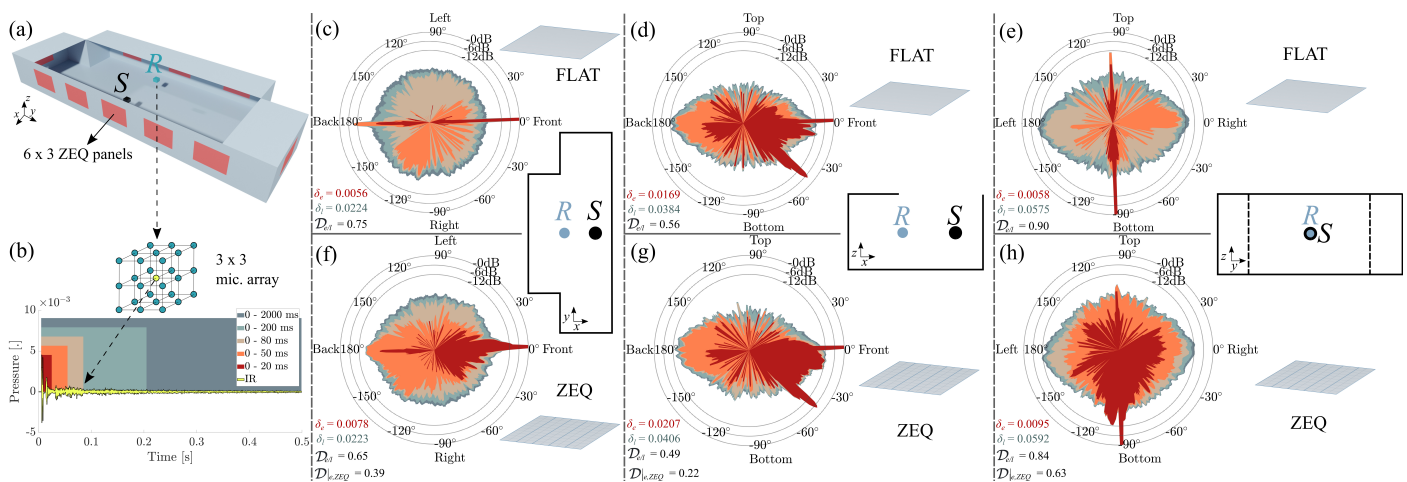
268 The scattering obtained with the QRD via FDTD is illustrated in Fig. 5(b), where  
 269 a strong temporal dispersion can be distinguished by the spreading of the scattered  
 270 waves through time. In such figure, one can see a major reflection shortly followed by  
 271 a similarly strong one, after which a series of multiple reflections appear with varying  
 272 frequency content and continuously less energy. This provides with a good illustration  
 273 of the scattering generated by the frequency-dependent behaviour of a sound diffuser.  
 274 The blue dots represent the absence of frequency content in very narrow time periods.  
 275 These are caused by wave interference due to the wavelength delay generated by the  
 276 phase-grating diffuser, providing with a time-frequency dispersion pattern.

277 Ultimately, Fig. 5(c) displays the scattered impulse response of the ZEQ obtained  
 278 through RLC circuit filtering. It can be observed that a strong temporal dispersion is  
 279 also obtained, with a similar pattern than the QRD. Even if the surface of the ZEQ is  
 280 flat, it reproduces a similar frequency-dependent behaviour than a QRD – although, as  
 281 mentioned previously, both temporal dispersions cannot be strictly compared one to the  
 282 other. Yet, the scattering from the QRD serves as a good reference to observe the added  
 283 temporal dispersion of the ZEQ.

## 284 5. Metadiffuser Equivalent Surface Impedance in a Large Space

285 For the purpose of this work, an orchestra pit is chosen for a large scene in which to  
 286 embed the proposed equivalent surface impedances in a 3D FDTD simulation. Half  
 287 the geometry of the orchestra pit of general dimensions  $[x,y,z](8,20,2.5)$  is idealized as  
 288 shown in Fig. 6(a), where a sound source  $S$  located at  $[x,y,z](2,10,1.5)$  and a receiver  $R$   
 289 located at  $[x,y,z](6,10,1.5)$  are highlighted. Note here that the pit is virtually isolated from  
 290 the exterior environment of what would be the rest of an opera house. The considered  
 291 orchestra pit is simulated following two different scattering strategies implemented on  
 292 the walls. In the first situation, no particular scattering on the boundaries is considered,  
 293 i.e., the walls are simply assumed perfectly rigid.





**Figure 6.** (a) Geometry of an ideal orchestra pit used in a 3D FDTD simulation. (b) Sample impulse response with different integration times used for the Spatial Decomposition Method (SDM). Spatio-temporal distributions of sound field energy ( $10 \log_{10} |p_s|$ ) for each coordinate plane in the orchestra pit received at location  $R$  from sound source  $S$  in (c–e) a pit with flat boundaries, and (f–h) a pit with sparsely distributed repetitions of equivalent surface impedance (ZEQ) patches.

294 The FDTD simulation grid resolution was set to 10.5 PPW at 8 kHz, resulting in  
 295 4.8 billion computational elements, in order to obtain a numerical dispersion errors less  
 296 than 1% [41] below such frequency. The simulations involving flat panels (no scatterers)  
 297 required 30 GB of memory computed in parallel using Nvidia CUDA spread over four  
 298 Nvidia Titan X GPU cards (Maxwell architecture). Simulations times with flat panels  
 299 were approximately 55 min for 0.5 s of simulated response. Including the more complex  
 300 RLC boundary conditions, the FDTD simulation took 65 min and required 3% more  
 301 memory running on the same GPUs. Thus, the equivalent surface impedance incurs  
 302 some extra minimal simulation costs (as expected from [29]), and it is also much smaller  
 303 relative to the simulation costs expected for a full-fledged multi-physics simulation  
 304 (taking into account QRM details and physics) in this space up to the chosen frequency  
 305 resolution.

306 The impulses responses captured within this environment are analysed by means of  
 307 a Spatial Decomposition Method (SDM) [42,43], which allows to determine the directions-  
 308 of-arrival (DOA) [44,45] of sound events in a 3D set of spatial impulse responses. The  
 309 latter are captured through a microphone array and can be windowed over different  
 310 integration times in order to show the evolution of the spatial sound field with respect  
 311 to time. In this case, a  $3 \times 3 \times 3$  virtual microphone array was used for recording the  
 312 numerical impulse responses at the receiver location, and is displayed in Fig. 6(b). For  
 313 data processing, the SDM Toolbox [46] made available by the Virtual Acoustics Team at  
 314 Aalto University, Finland, was used. The impulse responses cover a frequency range  
 315  $\Delta_f = [20 : 8000]$  Hz and are integrated over several incrementing time windows so that  
 316 the cumulative energy of the impulse responses can be observed through time. These  
 317 span from  $[0 - 20]$  ms to  $[0 - 2000]$  ms in order to cover most of the recorded information,  
 318 as shown in Fig. 6(b). Ultimately, the spatial sound field for each time window can be  
 319 plotted along the 3 orthonormal polar planes, i.e., lateral, transversal and median planes.

Figure 6(c) displays the spatio-temporal response at  $R$  in the transverse plane ( $xy$ -plane). It can be observed that early acoustic energy coming in the first 20 ms (red area) comes mostly from the front, where the sound source is located, with a significant contribution from the back as well due to the wall reflection. Later reflections integrated up to 2 s of the impulse responses (orange to blue areas) show an increase of sound energy for many directions of arrival due to a more chaotic state of sound reflections within the environment at those time steps, resulting in a relatively uniform angular late sound field distribution. Still, in most directions, the energy of the late sound field remains 12 dB or more below the initial energy recorded directly in the front and

in the back of the receiver. For both early and late spatio-temporal curves, a spatial autocorrelation coefficient for each time window can be estimated in a similar way to the diffusion coefficient in Eq. (3). In such manner, the closer the coefficient is to unity, the more uniform the spatial distribution. The ratio of the early to the late spatial autocorrelation coefficients can provide an early-to-late diffuseness coefficient [47],

$$\mathcal{D}_{e/l} = (1 - \delta_e / \delta_l), \quad (7)$$

where  $\delta_e$  and  $\delta_l$  are the early and late spatial autocorrelation coefficients, respectively. This formulation describes the rate of sound field isotropy between early and late integration times. In such case,  $\mathcal{D}_{e/l} \rightarrow 0$  implies that the evolution of the early-to-late diffuseness is non-existent, i.e., that both sound fields are identical, whereas  $\mathcal{D}_{e/l} \rightarrow 1$  indicates a maximum increase of isotropy between early and late diffuse sound fields, with the early sound field approximating that of a plane wave in free-field conditions and the late sound field approximating a spherical distribution.

In the absence of any sound diffuser, in the early [0 – 20] ms window, this results in an early autocorrelation coefficient  $\delta_e = 0.0056$ , while for the late time window of [0 – 2] s a value  $\delta_l = 0.0223$  can be seen. This shows that the early sound field is less uniform than the overall late sound field, which is to be expected in an environment where specular reflections of sound are dominant. In Fig. 6(c), an early-to-late diffuseness coefficient  $\mathcal{D}_{e/l} = 0.75$  is shown, illustrating a great increase in isotropy between the early and late diffuse sound fields. Similar observations can be made for the median ( $xz$ ) and lateral ( $yz$ ) planes in Figs. 6(d,e), respectively. In the median plane, an early-to-late diffuseness ratio  $\mathcal{D}_{e/l} = 0.56$  is achieved, showing less difference between early and late spatial distributions. This is supported by the open-air nature of the orchestra pit, where little extra reflection directions are enabled. In Fig. 6(e), a lower early-to-late diffuseness  $\mathcal{D}_{e/l} = 0.90$  can be identified for the lateral plane, bringing similar features than those encountered in the transverse plane, i.e., very narrow early spatial distribution significantly widening up in late integration times.

In the second pit configuration, an alternative scenario is proposed with clusters of  $6 \times 3$  repeated RLC fitted metadiffusers sparsely distributed along the walls. The intention behind this strategy is to distribute more sound energy in the early reflection regime of the pit, which incidentally may also help enhance the acoustic conditions required for musicians to experience a more suitable acoustical comfort while performing in such environment. The use of equivalent surface impedance is again motivated by the limiting constraints of modelling compact and detailed geometrical structures in a large 3D FDTD numerical scenery.

The above incentive is illustrated in Figs. 6(d-f) which show the spatio-temporal plots obtained in the second pit configuration for the transverse, median and lateral planes, respectively. In the transverse plane in Fig. 6(d), the early time integration area (red) demonstrates the arrival of strong reflections coming from broader directions than in the previous configuration with just rigid walls. This is supported by an increased autocorrelation coefficient  $\delta_e = 0.0078$ , which leads to confirm the presence of sound diffusers at the boundaries of the pit. A second major change in early sound distribution can also be seen for the [0 – 50] ms time window, displaying a much broader and homogeneous incoming sound field due to the presence of multiple 2<sup>nd</sup> and higher order reflections being more sparsely distributed within the pit thanks to the presence of the metadiffusers. Additionally, the late time integration area (blue) shows a very similar shape than in the previous scenario, with a value  $\delta_l = 0.0224$ . This implies that the late sound field obtained in both situations tends to a diffuse state of reflections with stochastic directions of arrival quite independently of any local scattering on the boundaries, which is here shown to only affects early sound distribution in a significant manner. The difference in early and late sound fields in Fig. 6(d) translates in a relative decrease of the early-to-late diffuseness coefficient compared to that of Fig. 6(a), with  $\mathcal{D}_{e/l} = 0.65$ . Likewise, a general increase of early-to-late diffuseness can be observed

367 in Figs. 6(e,f), with  $\mathcal{D}_{e/l} = 0.49$  and  $\mathcal{D}_{e/l} = 0.84$  in the median and lateral planes,  
 368 respectively. It is worth mentioning that the sound field in Fig. 6(d) shows a similar  
 369 sound field pattern compared to the one in Fig. 6(g), which is again due to the opening of  
 370 the pit limiting the potential directions of arrival for reflections in this particular section.  
 371 A small improvement to the early sound field distribution can however be seen between  
 372  $0^\circ$  and  $-45^\circ$ .

373 In addition to the early-to-late diffuseness, the more general diffuseness coefficient  
 374 [47]  $\mathcal{D}_e|_{ZEQ} = (1 - \delta_{ZEQ}/\delta_0)$ , can also be determined between the early sound fields in  
 375 both pit configurations, where the spatial autocorrelations obtained with homogeneous  
 376 flat boundaries are here considered as the most non-diffuse case of reference,  $\delta_0$ . In this  
 377 manner, a relative diffuseness,  $\mathcal{D}_e|_{ZEQ}$ , can be given for the different early sound fields  
 378 in each cross-section in order to provide with a more suitable measure of the impact of  
 379 sound scattering in the environment. In this sense,  $\mathcal{D}_e|_{ZEQ} \rightarrow 0$  means that both early  
 380 sound fields (in the homogeneous and ZEQ cases) have identical spatial distributions,  
 381 while  $\mathcal{D}_e|_{ZEQ} \rightarrow 1$  indicates a transition to a maximal isotropic distribution of the early  
 382 sound field generated in the ZEQ environment.

383 In Fig. 6(d), the latter results in a relative diffuseness coefficient  $\mathcal{D}_e|_{ZEQ} = 0.39$ ,  
 384 meaning that the presence of ZEQ panels helps increase the isotropy of the spatial  
 385 distribution at the receiver by a factor of 39% compared to that of the pit with homo-  
 386 geneous rigid boundaries. Similarly, relative diffuseness coefficients  $\mathcal{D}_e|_{ZEQ} = 0.22$   
 387 and  $\mathcal{D}_e|_{ZEQ} = 0.63$  can be observed in Figs. 6(e) and 6(f), respectively. These values  
 388 corroborate the analysis made so far in that the median plane in Fig. 6(e) shows only  
 389 a slight increase in early diffuseness between the two configurations, whereas a major  
 390 increase between early sound fields is displayed in the lateral plane in Fig. 6(f).

## 391 Conclusion

392 In this work, we have demonstrated the transposition of an acoustic metamaterial  
 393 (a metadiffuser) with intricate geometry into a simpler set of RLC circuit impedance  
 394 boundary conditions in order to compute the local physical conditions generated by the  
 395 metamaterial into a larger FDTD numerical environment. It has been shown that using a  
 396 novel phase-derivative zero-crossing fitting methodology, the impedances at the surface  
 397 of the metamaterial and those of the fitted RLC circuit equivalent surface impedance are  
 398 in excellent agreement. In addition, a good agreement between analytical and numerical  
 399 scattering, in space and time, generated by the RLC circuit boundary conditions has been  
 400 shown despite the drastic geometry reduction of the original metamaterial. Ultimately,  
 401 an ideal case study helped underline the impact of the local scattering generated by  
 402 the impedance boundary conditions into a practical situation, where the direct imple-  
 403 mentation of multiple metamaterials would have been forbiddingly taxing. The results  
 404 shown in this work demonstrate the advantages of simplifying complex metamaterial  
 405 structures for solving wave problems in global situations, without incurring significant  
 406 extra computational resources and time. This can be of great value in seismic, oceanic  
 407 or atmospheric wave propagation models which require extremely large volumes to  
 408 compute, as well as in critical environments where the metamaterial coverage becomes  
 409 significant, such as in transformation optics and room acoustics.

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