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## Determining ultrasonic propagation effective properties in complex heterogeneous media through microstructure-scale simulation

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### Abstract

Ray-based methods allow for fast computations of ultrasonic propagation in large components, and can be coupled with diffraction models to provide full simulations of NDE inspections. However, they do not account for complex interactions with highly heterogeneous propagation media, which can have a significant impact on inspection performances. In contrast, microstructure-scale finite element simulations consider these interactions but are too computationally intensive for large-scale simulations. The work presented in this communication aims at combining the advantages of these two approaches. On the one hand, finite element simulations for small volumes of the microstructure are used to determine parameters such as effective velocities, attenuations, and scattering coefficients. On the other hand, a ray-based model uses these data to compute wave propagation over distances that are large compared to both wavelengths and characteristic microstructure sizes. A dedicated simulation module has been implemented in a development version of the CIVA software. It generates random realizations of microstructures for given set of parameters, runs finite element computations, and post-processes their results to yield estimations of the properties of the macroscopic effective medium. The volumes considered by the finite element model are small enough to allow for 3D computations. Results were obtained for various types of microstructures, describing metals or concrete. This communication focuses on steel applications that were the focus of collaborative studies between CEA and EDF. The approach is promising, and contributes to bridging the gap between microstructure-scale modelling and larger scale simulations.

**KEYWORDS:** modelling, ultrasonic testing, heterogeneous medium, microstructure, finite element

### 1. Introduction

The scattering of ultrasonic waves in coarse microstructured material, such as some metals or concrete, can heavily affect inspections. The difference in scale between the microstructures and the wave propagation distances is a major challenge for modelling and simulation. A common approach is to consider only the coherent part of the ultrasonic



field, defined as the ultrasonic wave averaged over disorder. It behaves as if it propagated through a homogeneous effective medium that can be characterized, assuming it is isotropic, by a wave velocity and an attenuation for each propagation mode (longitudinal or transverse).

Historically, analytical models have been used to model the properties of the effective medium, for example by Stanke and Kino [1] for polycrystalline materials. Such models have limitations: they consider simple descriptions of the microstructure, which can limit their applicability, and they rely on approximations, which can cause inaccuracies. Another approach relies on finite element (FE) computations to simulate the propagation of plane waves through small volumes of the microstructure, and evaluate its attenuation and phase velocity [2]. As computational capabilities increase, this approach becomes more widely applicable but remains limited to small volumes representative of heterogeneous materials. In the case of the ultrasonic testing of large (with respect to the wavelengths considered) components, 3D numerical simulations at the microstructure scale are not feasible. In this context, identifying the properties of an effective medium can provide input to simplified models simulating the behaviour of the coherent wavefront. Among these models, solutions based on ray approaches [3] are well suited to large volumes and computationally efficient. The CIVA platform [4] relies on such methods for the simulation of ultrasonic bulk wave testing.

Tools dedicated to FE calculations in small representative elementary volumes (REV) have been added to the CIVA platform, with the aim of providing effective properties of materials based on their microstructures. A specific workflow has been set up to provide not only the average properties but also their variability in relation to the measured disparities. This communication presents an application of this approach to steel microstructure. In the longer term, the ambition of this work is to open these tools to CIVA users in its commercial version.

## **2. Finite element computations in small representative volumes**

The FE approach presented here is similar to the ones presented by several authors, including Van Pamel *et al.* [2] and Rzyz *et al.* [5]. This section gives a rough outline of the general approach and some specificities of the presented work.

### ***2.1 Geometry***

The computation domains are REVs defined as 3D grids describing the material properties of a given polycrystal. Based on periodic and equiaxed or elongated Voronoi tessellations, a tool to generate virtual microstructure has been implemented. It randomly generates the points of the Voronoi tessellation as well as the crystal orientations. Microstructures can also be imported under a .vtk format, which makes it possible to use output from other microstructure generation tools such as Neper [6] and DREAM.3D [7].

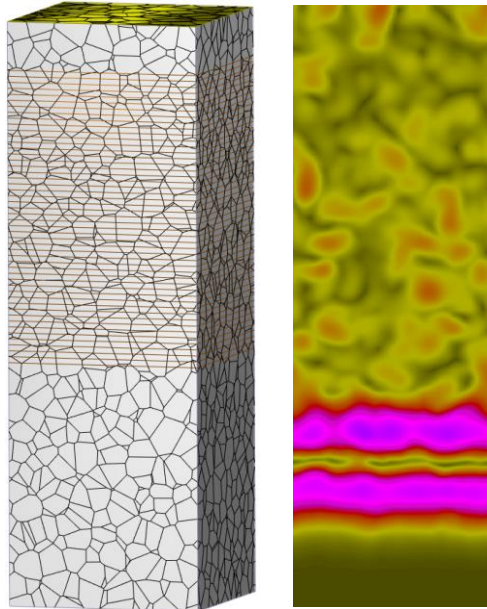
### ***2.2 Wave propagation simulations***

A Finite Element code dedicated to the simulation of ultrasonic wave propagation through heterogeneous microstructures was developed. It implements the elastodynamic

equations for a regular grid with low order elements. The weak form of the problem reads: for  $t > 0$  find  $u(t) \in \mathcal{V}$  such that  $\forall v \in \mathcal{V}$  we have

$$\frac{d^2}{dt^2} \int_{\Omega} \rho u \cdot v \, d\Omega + \int_{\Omega} C \varepsilon(u) : \varepsilon(v) \, d\Omega = \int_{\Gamma_z^+} f(t) \cdot v \, d\Gamma,$$

where  $\varepsilon$  is the strain,  $\mathcal{V}$  is the functional space of admissible ultrasonic displacement field,  $\Omega$  the domain of interest, and  $\Gamma_z^+$  is the upper boundary of the domain supporting a uniform normal stress  $f$  (generating an incident plane wave).  $\rho$  is the density and  $C$  is the constitutive law: their variations describe the microstructure. Periodic boundary conditions are imposed on the four interfaces tangent to the vertical propagation direction (left, right, front, back) which allows both quasi-longitudinal and quasi-transverse plane waves to propagate without boundary artefacts. The time marching algorithm is obtained after space discretization using conform low order finite element space and time discretization using an explicit “leap frog” time scheme. A graphical user interface was implemented in CIVA to set the input of the computation and to display the ultrasonic fields computed. An example is shown Figure 1.



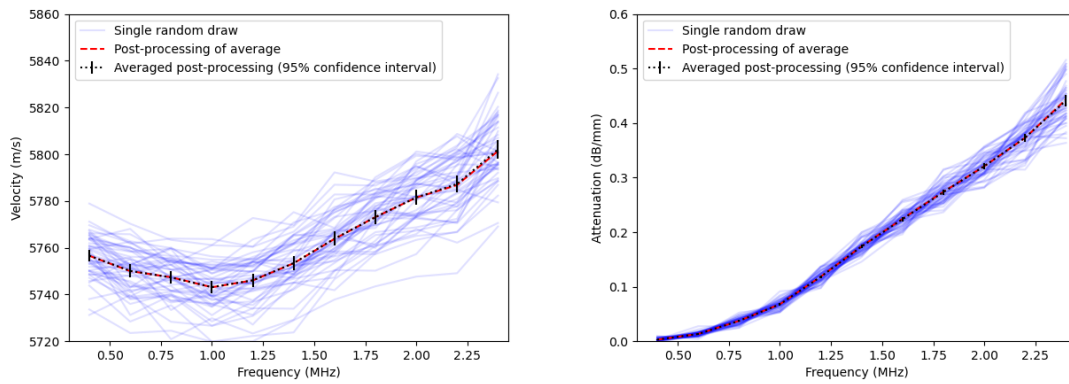
**Figure 1. Example of periodic elongated microstructure generated by a Voronoi tessellation, and cross-section of the ultrasonic field computed.**

### ***2.3 Post-processing***

Effective velocities and attenuation are computed automatically, using an approach similar to the one of Rzy *et al.* [5]. The properties of the coherent plane wave are obtained by averages over a series of horizontal planes (indicated by the orange lines left of figure 1). Its amplitude loss and phase shift as a function of depth yield respectively attenuation and velocity. These operations are performed in the frequency domain, and the results are obtained for a range of frequencies in the bandwidth of the source.

This procedure can be applied to a series of several random realizations of the same microstructure. The averages of the velocities and attenuations obtained can be calculated, along with the corresponding confidence intervals. It is also possible to average the

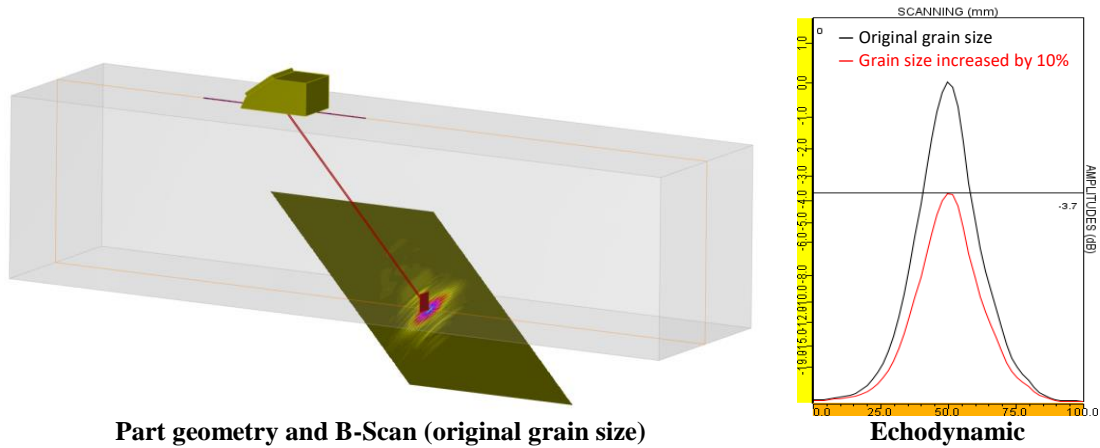
ultrasonic fields over all realizations before calculating a velocity and an attenuation. This second approach is more in line with the definition of an effective medium for a coherent wave, but does not allow for confidence intervals to be calculated. Figure 2 shows results obtained over 50 random realizations for the two approaches. The two averaging procedures yield similar results. These simulations are performed for volumes with dimensions  $10*10*30$  (mm), equiaxed, with one crystal per cubic mm. The material is steel with an  $8 \text{ g/cm}^3$  density, and cubic symmetry elastic constants defined by  $C_{11}=220 \text{ GPa}$ ,  $C_{12}=135 \text{ GPa}$ , and  $C_{44}=110 \text{ GPa}$ . The incident wave is longitudinal with a central frequency of  $1 \text{ MHz}$  and propagates during  $5 \mu\text{s}$ . With these parameters, the cell dimension is automatically set to  $0.16 \text{ mm}$ , for a total of  $742\ 203$  cells, and the time step is  $0.019 \mu\text{s}$ . The corresponding computation for one random realization requires less than one minute on a standard laptop.



**Figure 2. Examples of velocities and attenuations obtained for a steel model.**

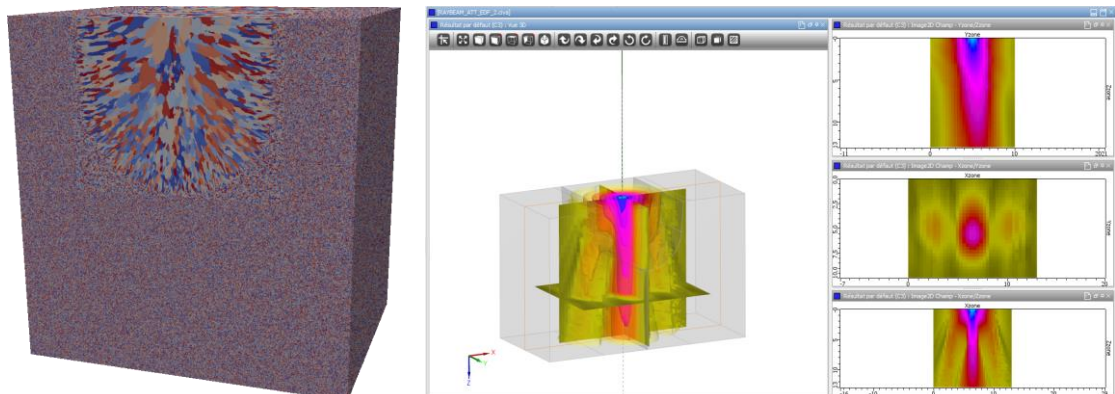
### 3. Fast computations for the effective medium

The effective velocities and attenuations can be used as entry for fast semi-analytical CIVA computations. Figure 3 shows an example of a simple computation of coherent wave performed based on the same parameters as figure 2. In this example, the material is considered homogeneous. Its velocities and attenuations are obtained by the post-processing of the averaged fields. It is a simulation of a scan over 50 positions with a  $1 \text{ MHz}$  transverse wave propagating for more than  $100 \mu\text{s}$  in a volume of several centimetres in all directions. For comparison, the computations have also been made with slightly increased grain sizes, which tends to increase attenuation and to decrease the magnitude of the echo. This approach only accounts for coherent waves, but has the advantage of being computationally efficient. Such scans would have taken weeks to compute for microstructure-scale finite elements, and take only seconds with the CIVA ray-based method.



**Part geometry and B-Scan (original grain size)**  
**Figure 3. Echo computations considering a coherent wave in an effective medium.**

Further works are in progress, more complex cases such as the example of figure 4. Two regions can be distinguished. The largest part of the sample can be considered as statistically homogeneous. The structure that is visible in the rest is a weld model. It can be described statistically as elongated crystals with continuous variations of sizes and orientation. The ultrasonic field presented here is a preliminary results obtained by considering an anisotropic medium with a continuous variation of orientation in the weld. Further works are in progress in order to compute the parameters of this medium with the REV approach.



**Figure 4. Crystallographic model of a weld in a steel sample, and ultrasonic field computed using the CIVA ray-based model.**

## 4. Conclusions

A FE simulation tool for the characterization of effective media has been implemented in a development version of the CIVA platform. It aims at providing input parameters for efficient ray-based computations. This approach combines fast large-scale computations with a precise accounting of small-scale microstructure effects.

The FE simulation tool can generate some simple microstructures, or import more complex ones generated by other software. An application to a weld model with large-scale microstructural variations is in progress, as presented in this communication. It is also being used to study ultrasonic propagation in dual-phase steel, using microstructures generated by the Neper software package.

In the current version of the approach, media are described by their ultrasonic velocity and attenuation. Additional parameters, such as coefficients quantifying structural noise, could be added in the future

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