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13. ABSTRACT (Maximum 200 words)

The objective of the effort was to develop mathematical algorithms and corresponding efficient numerical simulation tools for modeling propagation of acoustic waves through the human head, and, subsequently, to apply these tools to simulate energy transfer to the inner ear, and to assess the noise induced damage to the human hearing system.
The unique achievements/developments pertaining to this effort are: (i) adaptation of non-lossy, error controlled Fast Fourier Transform Adaptive Integral Method compression technique to the problems of acoustics, (ii) development of fast integral equation formulation for solving high-contrast problems (e.g. biological tissues embedded in air), (iii) parallel, distributed memory implementation of the developed algorithms with near perfect scalability, (iv) initiation of the extension of the developed approach to a full elasto-acoustic problem.
In summary, the developed fast, parallel, volumetric integral equation based solver is capable of accurate large-scale numerical simulations involving anatomically realistic models of a human head discretized with several million tetrahedral elements and characterized by complex geometrical details and large density contrasts.

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1 Objectives

The objective of our effort was

- to develop mathematical algorithms and corresponding efficient numerical simulation tools for modeling propagation of acoustic waves through the human head,

and, subsequently,

- to apply these tools to simulate energy transfer to the inner ear, and to assess the noise induced damage to the human hearing system.

2 Overview of the approach

It is a well established fact that integral-equation formulations provide the most accurate solutions to wave problems. They require, however, solving dense systems of linear equations. Traditional methods of solving such systems (e.g., through matrix inversion) are characterized by the computational complexity and memory requirements of the order of N^3. Here N is the number of unknowns, or a number of volume elements, necessary to resolve acoustic wave variations as well as geometrical details of the object. For complex, anatomically realistic models, N can easily become of the order of tens of millions. Hence, despite their reliability and accuracy, the conventional integral-equation based methods become computationally prohibitively intensive to provide solutions for realistic problems of interest.

During the last fifteen years a significant progress has been made in the development of *fast* frequency- and time-domain integral-equation solvers and, as a result, the ability of accurate and fast numerical simulations of wave propagation and scattering in complex media has dramatically improved. Matrix compression techniques, such as the Adaptive Integral Method (AIM)[1, 2], the Fast Multiple Method (FMM)[3], the pre-corrected FFT method[4], the sparse-matrix canonical grid method (SMCG)[5], have been developed. They allow solving large linear sets of equations with dense matrices utilizing storage and execution times characteristic of problems involving sparse linear systems. The physical idea behind such methods is that evaluation of interactions at large distances requires less resolution than at small distances. Consequently, the computational complexity and memory requirements of the compression methods scale approximately *linearly* with the number of unknowns N.

The underlying element of our approach is the Fast Fourier Transform (FFT) based AIM matrix compression method, initially developed in the context of electromagnetics for solving large-scale problems, and described in detail in Ref [2]. Adaptation of this formulation to large-scale acoustic problems was the initial step of our effort.

The main reason for choosing the FFT-based compression method rather than other compression techniques is that it provides superior efficiency in the treatment of both volumetric problems and sub-wavelength (tetrahedron size much smaller than the wavelength) discretizations. We note that sub-wavelength geometry regions constitute dominant portion of the head geometry model.

The final goal envisioned by us when undertaking this approach was

- to develop an efficient simulation tool capable to solve large-scale problems without compromising accuracy of the solution (due to the use of an integral equation based solver with non-lossy impedance matrix compression),
- to develop capability to work with geometries characterized by realistic geometrical details and material properties,

and thus to provide a numerical tool for modeling multiple physical mechanisms of acoustic energy transfer to the human ear and of assessing the noise induced damage.

3 Summary of the results

Our work comprised the following main efforts:

- development of fast integral equation based solver for acoustic wave propagation through inhomogeneous media,
- development of fast volumetric integral equation formulation for solving high-contrast acoustic problems (e.g., biological tissues embedded in air),
- a parallel, distributed memory implementation of the fast acoustic integral equation based solver,
- extension of the developed approach to elasticity.

The results of our work have been presented in two articles published in the Journal of Acoustical Society of America [8, 7]. Two additional papers, *Acousto-elastic integral equation based numerical simulation tools for analysis of sound wave interactions with human hearing system and design of high-noise protection devices* and *A parallel distributed-memory implementation of a fast acoustic integral-equation solver* are in the process of being submitted for publication.

The Sections below give the brief summary of the work performed.

3.1 Fast volumetric integral solver for acoustic wave propagation through inhomogeneous media

We adaptated the Fast Fourier Transform (FFT) based AIM matrix compression method,[1, 2] initially developed in the context of electromagnetics, to solving large-scale volumetric integral equations problems in acoustics.

In the AIM approach the original basis functions are expanded into sets of auxiliary, far-field equivalent, point sources located on nodes of a regular Cartesian grid. As the result, the far-field part of the interaction matrix becomes a Toeplitz matrix (or, more precisely, a product of a Toeplitz and sparse transformation matrices). The Toeplitz property allows computation of the matrix-vector product by means of FFTs with the $N \log N$ solution complexity. The near-field part of the interaction matrix is, by construction, sparse. Hence, its contribution to the solution complexity is of the order of $\mathcal{O}(N)$.

In comparison to other methods, we find the AIM fast solution scheme particularly suitable for solving acoustics problems. Its main advantage is that it can be applied to a wide frequency range – from tens of Hz to tens of kHz – with only a minor modification of the matrix compression scheme from the low- to high-frequency mode. (In the FMM approach, on the other hand, entirely different algorithms have to be used for low and high frequencies. The pre-corrected FFT method is less efficient than AIM at higher frequencies. Finally, for the considered applications, the cost of the SMCG method is significantly higher due to the necessity of computing a number of derivatives of the Green function.)

The developed algorithm makes possible simulations involving realistic geometries described in terms of a few million unknowns, characterized by highly sub-wavelength details, and large density contrasts.

Results of our work are presented in detail in [8]. Examples involving calculations of acoustic field distribution in a human head described in terms of approximately a million unknowns are also shown there.

3.2 Two-stage acoustic integral-equation solver

Conventional Lippmann-Schwinger integral equations, when applied to high-contrast problems (e.g. problems involving acoustically dense objects (biological tissues) immersed in a low-density medium (air)), may potentially become ill-conditioned.

An important feature of such high-contrast problems is the fact that most of the incident wave energy is reflected from interfaces between the low- and the high-density media, due to a large impedance mismatch between the materials. This circumstance does not cause computational problems in solving purely scattering problems, when these are formulated in terms of the boundary-element method, i.e., as surface integral equations involving boundary conditions on the surface of the scatterer. Difficulties, however, arise if one attempts to determine pressure distribution ***within*** an inhomogeneous body by means of the volumetric integral equations (the Lippmann-Schwinger equations). In this case, the fact that only a small fraction of the incident energy penetrates inside the scatterer causes the solution inside the object to be poorly determined. Mathematically, the integral equations describing the system become ill-conditioned: the solution is then strongly dependent on small changes in the incident field, and may become completely unreliable.

We developed a solution method which addresses the encountered difficulties. In the proposed approach an ill-conditioned high-contrast problem is solved in two stages: (1) in the first stage we solve the surface integral equation (as in boundary-element methods, although using volumetric elements); (2) in the second stage , we solve the volume problem with a modified incident field, defined in terms of the original field and the solution of the surface problem. Both the surface- and the modified volume problems are well conditioned. The procedure is rigorous, it does not involve expansions in the ratios of the material parameters, and it does not require alternating solving the surface and the volume equations (although each of the two problems may be, and usually is – for large systems – solved iteratively).

The approach is described in detail in [7].

3.3 Distributed-memory parallelization of the acoustic integral-equation solver

As we stated above, due to the utilization of the FTT based compression scheme, the computational complexity and memory requirements of our solver scale approximately linearly with the number of unknowns N. This allows for routine solutions of problems up to about 1,000,000 unknowns on a single processor system equipped with 4 GB memory.

However, in order to perform realistic large-scale simulations, involving tens of millions of unknowns, development of a parallel distributed-memory (MPI) code version which could run on a PC cluster with typical storage of about 2 GB memory per processor becomes essential.

Distributed memory parallelization of an integral equation based solver is highly nontrivial, since the nature of the algorithm gives rise a large amount of inter-processor communication. The three main computational stages to be considered in the parallelization process are:

(i) geometry processing and distribution of the geometry data,

(ii) construction of the stiffness matrix,

(iii) the iterative solution scheme.

A scalable parallel implementation of the solver requires that practically all geometry data are distributed across processors with a minimal, if any, replication. At the same time, during the construction of the stiffness matrix, processors must have access to some global geometry data in order to evaluate near-field couplings between sources and field variables assigned to different processors. We solve this problem by partitioning the geometry into non-overlapping slices and by assigning them to different processors. However, in the matrix construction stage, we temporarily assign several adjacent slices (of combined thickness equal at least to the near-field range) to each processor and "weld" them into a single stack. This welding procedure allows us to treat the entire stack of slices as a complete geometry, without having to introduce any additional connectivity data relating geometry elements in adjacent slices (which would have been necessary if slices were treated as separate geometries).

The most essential part of the algorithm is the FFT-based stiffness matrix compression and the associated fast matrix-vector multiplication procedure. The fact that Fourier transforms have to be evaluated in all three spatial directions requires a global rearrangement ("transposition") of the data and hence a large amount of inter-processor communication.

For these reasons we build the parallelization scheme of the code around the parallel FFT algorithm. We take here advantage of the availability of a widely used FFTW package [9], which allows operations on FFT data distributed spatially (in the form of "slices") across the processors. Its MPI-parallelized implementation is available in both the current version 3 and the previous version 2. We opted for the more recent MPI alpha version 3.2alpha3 (recently, in November 2008, this version has been replaced by 3.3alpha1).

However, a literal application of the FFTW routines would have been, in our case, inefficient. The equivalent cartesian-grid representation of sources and fields, used in our fast compression algorithm, requires zero-padding (with the index range extension by the factor of two in each direction) in order to eliminate aliasing in the discrete Fourier transformations, the conventional FFTW routines would locally operate on, and globally exchange, zero-filled buffers. Our application of the FFTW package allows a balanced distribution of the padding storage across the processors and reduces the amount of communication (the latter by avoiding sending and receiving zero or irrelevant padding data). Such an efficiency could not have been achieved by applying a single global FFT transformation from the package.

In spite of requiring a large amount of communication, the parallel FFT implementation in our solver achieves a nearly perfect scaling with the number of processors P (typically, a speedup by a factor about $P^{2/3}$ instead of the ideal speedup $\sim P$). We tested this behavior for up to several hundred processors.

The parallelization procedure implemented in the present code assumes a tetrahedral geometry discretization. However, it is applicable, with only minor modifications, to other types of geometry discretization (e.g., to node-based basis functions).

In Section 4 below we present some large scale simulations obtained with the parallel solver. We show solutions for a human head model, with and without a helmet, and with various materials used as padding in the space between the head and the interior helmet surface. The geometry models were discretized with approximately 10 million tetrahedra.

The parallelization procedure is described in detail in the attached draft of a manuscript, and will be submitted for publication.

3.4 Construction of the elasto-acoustic-solver

Our subsequent research effort focused on the construction of a full elasto-acoustic integral equation formulation and on the development of the related solver. In our work, we built on our experience acquired in the construction of a purely acoustic solver: in particular when overcoming difficulties associated with large contrast cases and strongly sub-wavelength contributions.

Three candidate versions of the solver were constructed:

- first order coupled acousto-elastic solver for the 4-dimensional unknown vector composed of three components of the displacement field $\mathbf{u}(\mathbf{r})$ and the pressure field $p(\mathbf{r})$,

- second order acousto-elastic solver for the 3-dimensional unknown vector composed of three components of the displacement field $\mathbf{u}(\mathbf{r})$,

- first order coupled acousto-elastic solver for the 9-dimensional unknown vector composed of three components of the displacement field $\mathbf{u}(\mathbf{r})$ and six (out of total nine) independent components of the stress tensor field $\hat{\tau}(\mathbf{r})$.

The above formulations differ in the relative content of either first or second order derivatives of material parameters, and in the treatment of high contrast contributions. At this point the choice of the numerically optimal formulation poses still an open question and more realistic calculations are needed to be carried out to answer it.

In addition to the listed above three candidate versions of integral equations formulations we also constructed a first order coupled acousto-elastic solver applicable to geometries composed of piecewise homogeneous regions. Such version of the solver involves exclusively unknown values of the traction field on interfaces between regions characterized by different Lame parameters λ, μ and the material density ρ. The main reason for devising such a method and constructing a surface integral equation solver was:

- to be able to model highly complex elements of the inner ear with surface elements,

- to quickly assess the importance of mechanisms contributing to energy transfer to the cochlea within the framework of a simplified but relatively realistic geometry model we constructed on a parallel STTR effort (we briefly describe the model in Appendix A below),

- to verify the validity of the purely volumetric integral equation solver (in addition to the analytic solution for a multi-layered elastic sphere we constructed on a parallel STTR effort).

As we noted, our choice of the optimal integral equation representation to be implemented in the final version of the elasto-acoustic solver remains still an open issue. However, we derived numerically expressions for matrix elements appearing in all of the candidate versions of the elasto-acoustic integral equations. In our derivations we used a new method of evaluation of integrals of kernel elements involving dipole terms of the Green function. The procedure offers both analytical simplicity and numerical accuracy. It does not require singularity extraction procedure since it reduces six-dimensional volumetric integrals to four-dimensional surface integrals with nonsingular integrands.

The derived expressions are applicable to linear basis functions on tetrahedral and triangular supports.

The article version of the approach described above is in preparation.

4 Examples

Pressure distributions in amultilayer sphere - comparison with the analytical solution. As the first example we present comparison of the results obtained with our solver with analytical solutions. Figs. 1 and 2 show results for the pressure distribution in a layered sphere, with the outer two shells chosen to represent skin and bone, and the interior of the sphere described by mechanical parameters of the brain tissue. The outer radius of the sphere is 14 cm, the thickness of the skin layer is 1 cm, and so is the thickness of the bone layer. The calculations employed a tetrahedral mesh with the tetrahedron sizes of about 2.8 mm; hence the thickness of the shell was about three times the tetrahedron size. The total number of tetrahedra is about $N = 5.5$ million.

Fig. 2 shows distribution of the absolute value of the pressure, $|p(\mathbf{r})|$, for the incident wave of frequency $f = 3\,\text{kHz}$).

Figure 1: Discretization of the layered sphere with $N = 5.5$ million tetrahedra.

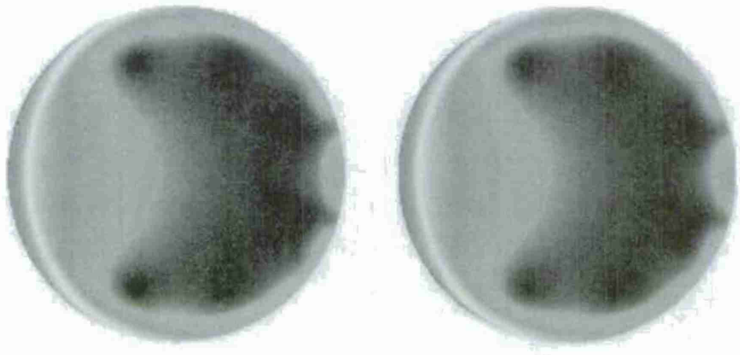


Figure 2: Distribution of the absolute value of pressure, $p(\mathbf{r})|$, on the plane passing through the center of the layered sphere, computed analytically (left) and by means of the described acoustic solver (right), for the discretization with $N = 5.5$ million tetrahedra.

The high quality agreement between the analytical results and code predictions for this high-contrast problem provides a support for the accuracy of our code.

Pressure distributions in a human head model in the presence and absence of a helmet. The next example involves a realistically shaped model of a human head and a model of helmet.

We assumed a steel helmet and the space between the helmet and the head filled either with air or with cork. In this computation we assumed the head model filled with a homogeneous material, with mechanical properties of bone. The models are placed in the field of a harmonic acoustic wave of frequency 5 kHz, incident laterally on the right ear of the head model. The corresponding wavelength in air is $\lambda = 6.8\,\mathrm{cm}$. Acoustic parameters of materials used in this and similar computations are listed in Table 1.

Geometries were discretized with tetrahedron sizes (edge lengths) of about 3 mm, resulting in (a) $N \simeq 2,700,000$ tetrahedra for the head, and (b) $N \simeq 4,700,000$ for the head and helmet system. The computations were carried out on a Linux cluster with the InfiniBand interconnect network, on 108 processors for the model (a) and 128 processors for the model (b). The total computation times were (a) about 50 minutes and (b) about 2 hours, the longer time for the case (b) due mostly to the larger number of iterations in the solution. One iteration required 4.6 s in the problem (a) and 6.6 s in the problem (b). We estimate that, in both cases, the overall computation time can be reduced by 30 to 50 % by optimizing the matrix construction stage of the code.

Table 1: Acoustic properties of materials used in the simulations

material	ρ/ρ_0	n^2
bone	1777.0	0.1524
brain	835.4	0.0564
cork	150.0	0.65
steel	6667.0	0.0035

Figure 3: Pressure distribution on the surface of the head in the absence of the helmet (left), pressure distribution on the surface of the helmet and the head with the space between the head and the helmet filled with air (center), pressure distribution on the surface of the head and the helmet with the space between the head and the helmet filled with cork (right).

Fig. 3 shows pressure distribution on the surface of the head in the absence of the helmet, as well as pressure distributions on the surface of the helmet and the head with the space between the head and the helmet filled with air and cork respectively. In all cases we observe a surface wave being formed on the geometry exterior.

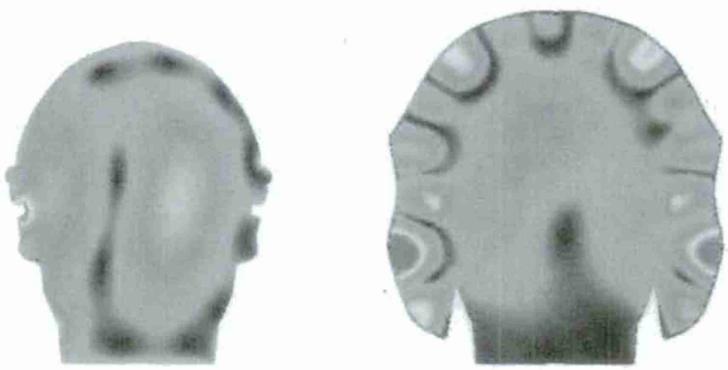
In Fig. 4 we show pressure distribution inside the human head model in the presence and in the absence of a helmet.

The results show a nontrivial behavior of the solutions and exhibit physical phenomena which may be relevant in the design of protective devices.

In the case of the head, Fig. 4(a), the pressure is maximal at the entrance to the ear canal, and it is relatively smoothly distributed inside the head. In fact, the solution is suggestive of a resonance-type (P-wave) behavior: the pressure changes sign along the approximately vertical line seen in the Figure.

The solution for head and helmet system, Fig. 4(b), is quite different. It exhibits a distinct oscillatory behavior along the surface of the helmet and in the region filled by cork. This region appears to have properties of a "waveguide'. Because of the cork density being significantly lower than that of the surrounding materials (the helmet and the head), and the resulting impedance mismatch at the boundaries, the wave tends to be trapped in that region. Since the refractive index of cork is not much different from that of air, wave oscillations are relatively rapid. We stress, however, that the physical picture suggested by Fig. 4(b) would change if we included dissipative (attenuation) effects in the filling material, e.g., if we considered a strongly damping porous material characterized by a complex refractive index.

We also note that, for the particular frequency considered here, the presence of a helmet completely changes the pressure distribution in the head, but does not reduce its maximum value (the data in Fig. 4(a) and Fig. 4(b) are plotted in different scales).



(a) (b)

Figure 4: Pressure distributions in the coronal plane for (a) the human head model and (b) the system consisting of the human head and a steel helmet models, with the in-between space filled by cork. The models are subject to an acoustic wave of unit pressure amplitude and frequency 5 kHz, incident from the left. The maximum pressure value is about 4 in (a) and 15 in (b).

5 Appendix A: Test model of a human head

On a parallel STTR, Phase II effort, we constructed a test model of a human head. The model consists of a skin, skull and brain tissue, with the cochlea embedded in the skull. In addition, we also constructed a model of a helmet and a padding material placed between the head and the interior of the helmet surface. The components of the head model are shown in Figs. 5. The helmet model is shown in Fig. 6.

The above elements constitute a minimal yet relevant set of geometry components required in carrying out simulations of energy deposited within the cochlea region and, subsequently, in the determination of auditory effects of the propagating wave. The helmet geometry allows us to investigate the influence of the padding material, as well as of possible air gaps between the head and the helmet structure on the energy distribution inside the head model.

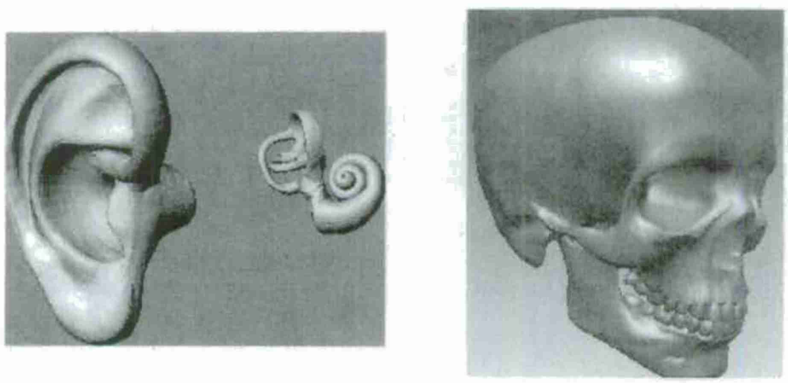


Figure 5: The external ear, the cochlea, and the skull models used in the simulations.

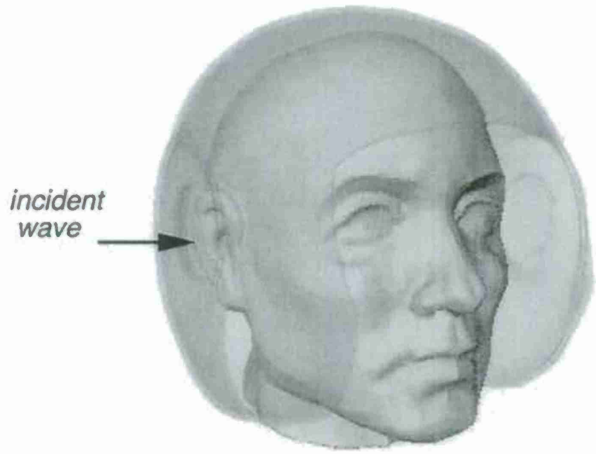


Figure 6: Model of the external head surface and the helmet. The arrow indicates the direction of the incident wave.

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