

OptimUS: An open-source Python library for solving 3D acoustic wave propagation

We are happy to announce the first release of OptimUS, an open-source Python library for simulating linear acoustic wave propagation in an unbounded domain with multiple homogeneous scatterers.

Background

Initial development of OptimUS started with research funded by EPSRC grant EP/P012434/1, the aim of which was to develop a novel mathematical framework for optimising patient specific treatment plans for ultrasound ablative therapies in the abdomen. A key milestone of this research was to significantly reduce the computational footprint associated with 3D biomedical ultrasound problems, disseminating fully tested and validated code in an open-source and user-friendly package.

Features

OptimUS solves the Helmholtz transmission problem using the boundary element method (BEM). The main features of OptimUS are:

- Easy workflow to define, solve, visualise and export the results of 3D acoustic wave propagation problems
- Accurate and efficient BEM formulations at large ka and at material interfaces with large contrasts in density and speed of sound
- Efficient parallelised calculation of fields emitted from different acoustic sources such as plane waves, point sources, as well as planar, focused, single-element and array transducers
- Rapid prototyping within a user-friendly environment, using Jupyter notebooks.
- Simulations can mostly be performed on desktop machines while large-scale experiments run on high-performance nodes.

Method

OptimUS works entirely in the frequency domain. Hierarchical matrix compression techniques [1, 2] and dedicated preconditioners [3] significantly reduce the memory footprint and increase the convergence rate of iterative solvers. Acoustic transmission problems across high-contrast media can be efficiently and accurately solved for high ka scenarios [4].

A distinct advantage of the BEM is that it does not suffer from numerical dispersion or domain truncation effects. Furthermore, acoustic sources and domains are not restricted by a Cartesian grid, thereby eliminating staircasing effects commonly associated with other numerical schemes such as finite-difference time domain methods.

Applications

OptimUS has been used for a wide range of biomedical problems in the field of therapeutic ultrasound (see Figures 1 and 2). More broadly, our software library will be of particular interest to researchers using or developing computational acoustics, especially within the following UKAN+ Special Interest Groups:

- Biomedical Ultrasound
- Computational Acoustics
- Mathematical Analysis in Acoustics

- Underwater Acoustics

OptimUS can also be used as a pedagogical tool at undergraduate and postgraduate levels.

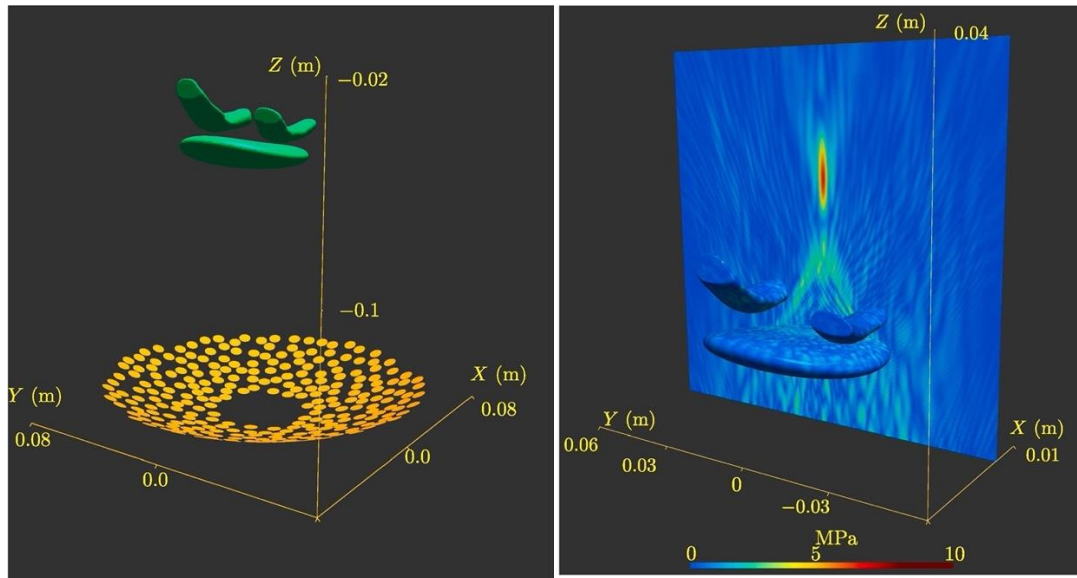


Figure 1. (a) Schematic diagram of the focused ultrasound array, an abdominal fat layer and two ribs, (b) calculated absolute value of the total pressure at 1 MHz. See reference [2] for more information.

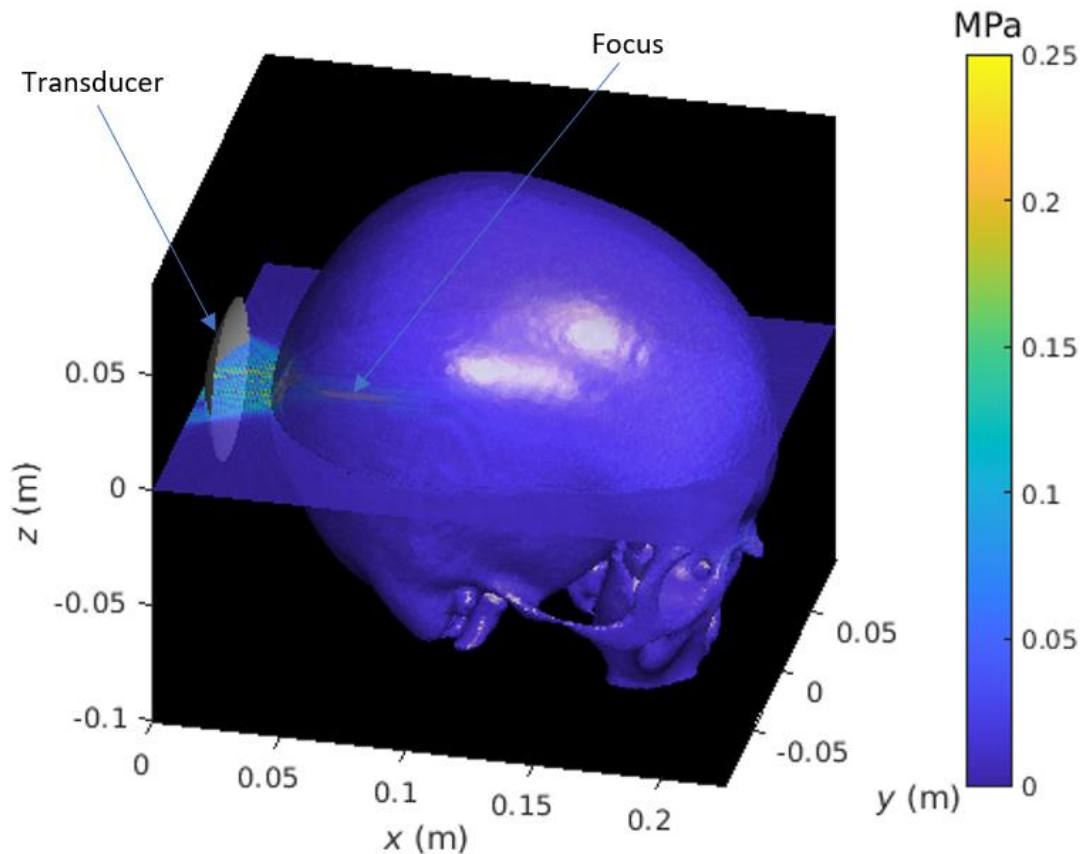


Figure 2. Ultrasonic pressure field predicted by OptimUS for a single-element focused transducer at 0.5 MHz. Cranium immersed in water. See reference [5] for more information.

Repository and contact information

Check out the GitHub repository page for further details on how to access and use OptimUS:

<https://github.com/optimuslib/optimus>

Feel free to contact the OptimUS team (on GitHub or via email: optimusproject2017@gmail.com) should you require further information.

We welcome feedback, new collaborations and contributions from the UKAN+ community to further develop OptimUS.

On behalf of the OptimUS team,

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References

- [1] E. van 't Wout, P. Gélát, T. Betcke, and S. Arridge, "A fast boundary element method for the scattering analysis of high-intensity focused ultrasound," *J. Acoust. Soc. Am.* **138**(5), 2726–2737 (2015).
- [2] W. Śmigaj, S. Arridge, T. Betcke, J. Phillips & M. Schweiger, "Solving boundary integral problems with BEM++," *ACM Trans. Math. Softw.* **41**(2) 6:1–6:40 (2015).
- [3] S. R. Haqshenas, P. Gélát, E. van 't Wout, T. Betcke, and N. Saffari, "A fast full-wave solver for calculating ultrasound propagation in the body," *Ultrasonics* **110**, 106240 (2021).
- [4] E. van 't Wout, S. R. Haqshenas, P. Gélát, T. Betcke, and N. Saffari, "Boundary integral formulations for acoustic modelling of high-contrast media," *Comput. Math. Appl.* **105**, 136–149 (2022).
- [5] J. F. Aubry, O. Bates, C. Boehm, K. B. Pauly, D. Christensen, C. Cueto, P. Gélát, L. Guasch, J. Jaros, Y. Jing, R. Jones, N. Li, P. Marty, H. Montanaro, E. Neufeld, S. Pichardo, G. Pinton, A. Pulkkinen, A. Stanzola, A. Thielscher, B. Treeby, and E. van 't Wout, "Benchmark problems for transcranial ultrasound simulation: Intercomparison of compressional wave models," *J. Acoust. Soc. Am.* **152**(2), 1003–1019, 2022.