ALGEBRAIC ERROR BOUNDS AND STOPPING CRITERIA IN FFT-BASED HOMOGENIZATION SOLVERS

Nachiketa Mishra¹, Jaroslav Vondřejc² and Jan Zeman^{3*}

¹International Center for Theoretical Sciences, Bangalore, India, nachiketamishra@icts.res.in ²Technische Universität Braunschweig, Mühlenpfordtstrasse 23, D-38106 Braunschweig, j.vondrejc@tu-braunschweig.de

³Czech Technical University in Prague, Thákurova 7, 166 29 Prague 6, jan.zeman@cvut.cz

Key words: Homogenization, Spectral methods, Discretization and algebraic errors, Conjugate gradient methods, Quadrature-based error bounds

This talk concerns error analysis of iterative FFT-based homogenization solvers introduced to the field of computational homogenization in the seminal work by Moulinec and Suquet [1]. Our particular focus in on the Fourier-Galerkin method with exact integration combined with the projected Conjugate Gradient (CG) algorithm, because this combination yielded the most accurate results in our recent study [2].

Following the exposition by Papež at al. [3], we show that the total error splits into mutually orthogonal *discretization* and *algebraic* parts. The discretization error arises from the Galerkin projection on a sub-space of trigonometric polynomials and can be bounded, e.g., by duality techniques developed in [4]. Besides, thanks to the sharp estimates on the extreme eigenvalues of the system matrix [2], the algebraic error can be rigorously estimated by quadrature-based bounds by Meurant and Tichý [5] that exploit the specific structure of iterates generated by CG. The performance of the latter bounds is demonstrated using selected examples. Furthermore, we show that the number of CG iterations can be significantly reduced using stopping criteria that balance discretization and algebraic errors.

Acknowledgments. This work was supported by the GAČR–DFG project No. 17-04150J.

REFERENCES

- [1] Moulinec, H. and Suquet, P. A fast numerical method for computing the linear and nonlinear mechanical properties of composites, C. R. Acad. Sci. Paris (1994) **318**, pp. 1417–1423.
- [2] Mishra, N. and Vondřejc, J. and Zeman, J. A comparative study on low-memory iterative solvers for FFT-based homogenization of periodic media. J. Comput. Phys. (2016) 321, pp. 151–168.
- [3] Papež, J. and Liesen, J. and Strakoš, Z. Distribution of the discretization and algebraic error in numerical solution of partial differential equations. *Linear Algebra Appl.* (2014) 449, pp. 89–114.
- [4] Vondřejc, J. and Zeman, J. and Marek, I. Guaranteed upper-lower bounds on homogenized properties by FFT-based Galerkin method. *Comput. Methods Appl. Mech. Eng.* (2015) 297, pp. 258–291.
- [5] Meurant, G. and Tichý, P. On computing quadrature-based bounds for the A-norm of the error in conjugate gradients, Numer. Algorithms (2013) 62, pp. 163–191.