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On the application of Fast Multipole Methods to Helmholtz problems with complex wavenumber

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The Fast Multipole Method (FMM) is in particular applied to many physical problems governed by equations of Helmholtz type which arise for e.g. linear acoustics, electromagnetic or elastic waves upon using Fourier transform in time or applying excitations under prescribed-frequency conditions. All cases involve integral equations whose (scalar or tensorial) kernels are defined, for three-dimensional formulations, in terms of the fundamental solution $K(\mathbf{r}) = \exp(ikr)/4\pi r$ and its derivatives. The FMM crucially rests upon expansions of $K(\mathbf{r})$ that allow a separation of variables between the “field” point \mathbf{y} and the “source” point \mathbf{x} (with $\mathbf{r} = \mathbf{y} - \mathbf{x}$), which are available in several forms. These include the multipole expansion, based on the Gegenbauer addition theorem, and the plane-wave expansion of $K(\mathbf{r})$ in diagonal form. For real values of the wavenumber k , which correspond to wave propagation problems in lossless media, FMMs based on either type of expansion have been extensively studied and implemented. These studies have in particular established that multipole expansions of $K(\mathbf{r})$ are too costly except at low frequencies (because the expansion truncation threshold increases with k), while plane-wave expansions are well-suited to higher frequencies but break down in the low-wavenumber limit. It is also known that in the zero-wavenumber limit (i.e. static problems) an a-priori indication on the number N of multipoles to be employed in truncated expansions in order to obtain a prescribed accuracy in $K(\mathbf{r})$, unaffected by the dimensions of the cells in the octree, is usually available. This nice feature (which ensures a $O(n_{\text{dof}})$ complexity per iteration for multi-level FMMs applied to static problems) is no longer present in frequency-domain applications ([5, 1, 2]), where the implementation of the method is substantially complicated by the need to adapt the truncation order to the level of the octree (resulting in a $O(n_{\text{dof}} \log n_{\text{dof}})$ complexity per iteration). In contrast, only scattered efforts so far have been devoted to FMMs for Helmholtz-type problems involving *complex* wavenumbers k . Such formulations involve wavenumbers of the form $k = (\alpha + i\beta)\vartheta$ (where ϑ is a parameter related to frequency and α, β are real constants). The paucity of available studies notwithstanding, complex-wavenumber FMMs arise for a number of different physical problems. First, such equations and kernels arise naturally upon considering wave propagation in lossy media (e.g. soils) in which mechanical or electromagnetic waves are damped. Such materials (e.g. viscoelastic materials) may be described, within frequency-domain approaches, in terms of linear constitutive relations involving complex moduli. This leads to complex-valued wavenumbers such that $0 < \beta < \alpha$, often with a small imaginary part, i.e. such that $\beta/\alpha \ll 1$, and represents the most direct generalization of Helmholtz-type equations with real wavenumbers. Another class of such problems correspond to parabolic problems involving elliptic partial differential operators in the space variables and first-order time derivatives, upon using Fourier transform in time or applying excitations at a prescribed frequency. They include heat conduction, transient Stokes flows, and eddy currents, and the associated Green’s functions or tensors involve $K(\mathbf{r})$ with $\alpha = \beta = 1$. Transient Stokes flows arise e.g. in connection with the analysis of dissipation in Micro-Systems. Also amenable to the general framework of Helmholtz-type equations (with purely imaginary frequency) is the computation of Casimir forces, which are attractive force arising between uncharged conductive surfaces in vacuum, a remarkable consequence of quantum electrodynamics. In spite of its complicated nature, this phenomenon is now acquiring technological importance, as it has a major role in modern micro- and nano-technologies.

Finally, one may mention that optical tomography also leads to a Helmholtz equation with complex wavenumber (defined in terms of modulation frequency of light and optical parameters of the medium), this time such that $\beta < 0 < \alpha$ and $|\beta| < |\alpha|$. The above-summarized wealth of different applications justifies an investigation of the Fast Multipole Methods for this class of problems. Currently, little is known about e.g. the appropriate non-dimensional frequency ranges of applicability of either multipole-based or plane wave-based expansions, or the choice of truncation order. In this article, an empirical study of multipole expansions of $K(\mathbf{r})$, of the kind known to be suitable for low real wavenumbers, is conducted for complex wavenumbers of the form $k = (\alpha + i\beta)\vartheta$, so as to estimate ranges of applicability in terms of ϑd (D denoting a characteristic cell size) and suitable settings for the truncation order N according to the values of α, β .

Empirical rules trying to estimate the truncation order N to be employed in the Gegenbauer addition formula (see e.g. [5]) do not take into account that $K(\mathbf{r})$ decays exponentially with $\|\mathbf{r}\|$ if $\beta > 0$. For this reason, the relative accuracy E_N achieved on $K(\mathbf{r})$ may not be the most useful indicator, as it does not take into account the absolute relevance of the contribution of field points far from the collocation in the presence of dissipative terms. For this reason, an alternative line of reasoning is proposed. Since for large values of $\beta\vartheta r$ the decaying term dominates, it is natural to investigate the relative kernel error in a way that takes into account the absolute contribution of the kernel to the overall evaluation of integral operators. This suggests to consider the pointwise weighted error

$$E_M = E_N \exp^{-\beta\vartheta 2d} \quad (1)$$

instead of the standard relative error E_N , where d is half-size of the leaves in the octree. It is found that for $|\alpha| \leq \beta$ the largest weighted error occurs at $\vartheta d = 0$ and, for instance, $N = 12$ guarantees $\log(E_M) = -6$ while $N = 8$ is sufficient for ensuring $\log(E_M) = -4$. For $\beta < |\alpha|$ one can still identify the truncation order N such that E_M is controlled and less than a prescribed amount, independently of ϑd , but this threshold now depends on β . It is found that $\log(E_M) = -6$ or $\log(E_M) = -4$ can be achieved using N_6 and N_4 terms, respectively, with:

$$N_6 = 10.1 + 1.68\beta^{-1.4} \quad (2)$$

$$N_4 = 6.7 + 1.15\beta^{-1.4} \quad (3)$$

$$N_3 = 5.28 + 0.65\beta^{-1.5} \quad (4)$$

The above empirical formulas are valid for $0.1 \leq \beta \leq 1$.

From some simple tests performed it is apparent that the same accuracy can be expected on full scale problems.

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