A Novel Approach for Fast Evaluation of 1-D and 2-D Infinite Summations

E. P. Karabulut[1], *V. B. Ertürk*[2], *S. Adanır*[3], *L. Alatan*[3], and *M. I. Aksun*[1]

[1] Koc University, 34450 Sariyer Istanbul, Turkey, ekarabulut@ku.edu.tr, iaksun@ku.edu.tr

[2] Bilkent University, 06800 Bilkent Ankara, Turkey, vakur@ee.bilkent.edu.tr

[3] Middle East Technical University, 06531 Ankara, Turkey, sadanir@aselsan.com.tr, lalatan@metu.edu.tr

In many engineering applications, relatively difficult infinite summations with quite complex terms need to be computed numerically. These applications may include the calculation of free-space or planar-media periodic Green's functions in electromagnetics (EM), the determination of the electrostatic energy of ionic crystals in chemistry and the nucleic acid simulations in molecular dynamics. The difficulty of such computations usually arises from the fast oscillatory and slowly convergent nature of the summations. For instance, the EM analysis of cylindrical geometries may require the computation of slow convergent infinite summations of cylindrical Hankel and Bessel type functions; in numerical simulations of periodic structures, e.g. in the analysis of antenna arrays and photonic band gap materials, the periodic Green's functions need to be calculated for each impedance matrix elements in the method of moments, requiring the evaluation of many infinite summations of complex functions to fill in the entire matrix.

In this study, a novel method is proposed to compute slowly convergent summations. In principle, the idea of the method is as follows: if one i) takes a sufficient series of partial sums, and ii) considers them as a set of data, and iii) approximates the data as a sum of complex exponentials, the DC term (the residue of the exponential with zero complex pole) of this approximation would be the result of the summation of interest. The method is quite efficient and robust because of the fact that the partial sums of an infinite summation always exhibit an oscillating behavior, and if the summation is convergent, the oscillation dies out eventually and leads towards a DC term, which is the result of the summation. Therefore, the partial sums are approximated in terms of exponentials to find this zero frequency term. In order to approximate the data as a series of complex exponentials, a subspace approach called the generalized pencil of function (GPOF [1]) is employed. For the sake of demonstration, the method is first applied to a 1-D problem with a known analytical result, and its performance is compared to the direct summation in terms of the computation time. Then, the free-space periodic Green's function (FSPGF) is computed by the proposed method, for its verification in 2-D summations, and the results are compared with those obtained by the Ewald method [2]. It should be noted that, the proposed method can also be applied to 1-D and 2-D slowly convergent infinite *integrals* by converting them into infinite summations. Since the main idea is the same, once a sufficient set of partial integrals is obtained, the rest of the algorithm becomes exactly the same. However, for the sake of coherence and brevity, no examples on integrations are provided in this study.

References

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