KRYLOV SUBSPACE BASED ACCELERATION STRATEGIES FOR THE SOLUTION OF HIGH-FREQUENCY MULTIPLE SCATTERING PROBLEMS

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Abstract

A recently developed integral equation method can deliver scattering returns with prescribed error tolerances in fixed computational times for single-scattering problems of arbitrarily high frequency. To encompass multiple-scattering effects while preserving a frequency independent operation count, recent extensions of the approach are based on a spectrally convergent Neumann series to decompose the overall scattering return into a superposition of single-scattering contributions. For cases wherein the series is slowly convergent, these implementations have relied on analytic continuation mechanisms (Padé approximation) to reduce the number of iterations necessary to reach a prescribed error tolerance. Here, we present a new Krylov-subspace method that provides a further significant reduction in the number of iterations while still retaining the frequency-independent computational cost.

Introduction

Oscillatory problems, such as those that arise in connection with acoustic, elastic or electromagnetic simulations, have provided significant impetus to the design of advanced numerical algorithms for decades and particularly over the last twenty years. As a result, an array of sophisticated simulation schemes (based on e.g. finite elements, finite differences, multi-resolution analyses or boundary integral equations) have been devised to efficiently tackle these applications. Today, such algorithms enable the virtual analysis of large practical configurations that may span up to a few hundred wavelengths. The very nature of these approaches, however, limits their applicability at higher frequencies since the numerical resolution of field oscillations translates to a commensurately higher number of degrees of freedom and this, in turn, can easily lead to impractical computational times.

A recently developed scattering simulator (based on the *rigorous* solution of integral equation formulations which incorporate asymptotic phase information), on the other hand, has demonstrated the capability of delivering solutions in prescribed error tolerances within fixed computational times for single-scattering problems of arbitrarily high frequency [1]. To encompass multiple-scattering effects, recent extensions of the approach are based on the iterated evaluation of a suitable Neumann series that reduces the overall problem to a sequence of single-scattering events. This series converges spectrally, with a rate that can be asymptotically determined; see [2–4]. As such it is amenable to acceleration via Padé approximation, and use of this latter technique can be shown to provide a substantial reduction in the number of iterations to reach a prescribed tolerance. Here, we present a new Krylov-subspace method that provides a further significant reduction in the number of iterations while still retaining the frequency-independent operation count.

High-frequency Multiple Scattering Formulation

For simplicity of presentation, we consider here the (exterior) sound soft acoustic scattering problem from a bounded obstacle $K \subset R^n$ $(n = 2, 3)$

$$\begin{cases} \Delta u(x) + k^2 u(x) = 0, & x \in R^n \backslash \overline{K}, \\ u(x) = -u^{\rm inc}(x) = -e^{ik\alpha\cdot x}, & x \in \partial K, \\ \lim\limits_{|x|\to\infty} |x|^{(n-1)/2} \left[\left(\frac{x}{|x|}, \nabla u(x) \right) - iku(x) \right] = 0 \end{cases}$$

and recall that its solution can be recast, through the use of Green's identities, in the form of an integral equation

$$\eta(x) - \int_{\partial K} \frac{\partial G(x,y)}{\partial \nu(x)} \, \eta(y) \, ds(y) = 2 \, \frac{\partial u^{inc}(x)}{\partial \nu(x)} \qquad (1)$$

for the (unknown) *physical* quantity η (normal velocity of the total field in acoustics) confined to the scattering surface ∂K where $G = -2\Phi$ and Φ is the outgoing fundamental solution to the Helmholtz equation. When the scatterer is composed of several (disjoint) substructures $K = \cup\{K_\sigma : \sigma \in \mathcal{I}\}$, equation (1) can be written as

$$(I - R)\eta = f \qquad (2)$$

where $f = [f_{\sigma_1}, \ldots, f_{\sigma_{|\mathcal{I}|}}]^t$, $f_\sigma = 2\partial u^{inc}/\partial\nu|_{\partial K_\sigma}$, $\eta = [\eta_{\sigma_1}, \ldots, \eta_{\sigma_{|\mathcal{I}|}}]^t$, $\eta_\sigma = \eta|_{\partial K_\sigma}$ and the operator R is defined for $x \in \partial K_\sigma$ as

$$(R_{\sigma\tau}\eta_\tau)(x) = \int_{\partial K_\tau} \frac{\partial G(x,y)}{\partial \nu(x)} \, \eta_\tau(y) \, ds(y) \, .$$

Inverting the diagonal part of the equation in (2) yields

$$(I - T)\eta = g \tag{3}$$

where $g_\sigma = (I - R_{\sigma\sigma})^{-1} f_\sigma$, $T_{\sigma\tau} = (I - R_{\sigma\sigma})^{-1} R_{\sigma\tau}\delta_{\sigma\tau}$ and δ is the Kronecker symbol. Considering the series solution to (3)

$$\eta = \sum_{m=0}^{\infty} \eta^m = \sum_{m=0}^{\infty} T^m g\,,$$

we note that

$$\eta^m\big|_{K_{\sigma_m}} = \sum_{\substack{\sigma_0,\ldots,\sigma_{m-1}\in\mathcal{I} \\ \sigma_j\neq\sigma_{j-1}}} T_{\sigma_m\sigma_{m-1}} T_{\sigma_{m-1}\sigma_{m-2}} \cdots T_{\sigma_1\sigma_0} g_{\sigma_0}\,, \tag{4}$$

for each $\sigma_m \in \mathcal{I}$, and each summand in (4) corresponds, in the limit of infinite frequency, to a group of rays that reflect through $\partial K_{\sigma_0}, \ldots, \partial K_{\sigma_{m-1}}$ and arrive at ∂K_{σ_m}. Thus the phase $\varphi_m(x)$, for $x \in \partial K_{\sigma_m}$, of the corresponding summand can be evaluated a priori as

$$\varphi_m(x) = \alpha \cdot x^{m,0}(x) + \sum_{j=0}^{m-1} |x^{m,j+1}(x) - x^{m,j}(x)|$$

where the points

$$(x^{m,0}(x), \ldots, x^{m,m-1}(x)) \in \partial K_{\sigma_0} \times \cdots \times \partial K_{\sigma_{m-1}}$$

satisfy the law of reflection throughout to finally arrive at $x^{m,m}(x) := x \in \partial K_{\sigma_m}$. Knowledge of the phases φ_m, in turn, allows for their extraction in the recursive application of the operators $T_{\sigma\tau}$ and thus for the fast, frequency independent, evaluation of the latter. In more detail, for a given sequence $\{\sigma_m\}_{m\geq 0} \subset \mathcal{I}$ with $\sigma_m \neq \sigma_{m+1}$, letting

$$\eta_0 = g_{\sigma_0} \quad \text{and} \quad \eta_m = T_{\sigma_m\sigma_{m-1}}\eta_{m-1}\,,\ (m \geq 1)$$

we have $\eta_m = \eta_m^{\text{slow}} e^{ik\varphi_m}$, and thus

$$\eta_m^{\text{slow}} - e^{-ik\varphi_m} R_{\sigma_m\sigma_m}(e^{ik\varphi_m}\eta_m^{\text{slow}}) = F^{\text{slow}} \tag{5}$$

where

$$F^{\text{slow}} e^{ik\varphi_m} = R_{\sigma_m\sigma_{m-1}}(e^{ik\varphi_{m-1}}\eta_{m-1}^{\text{slow}})$$

is twice the normal velocity of the field scattered off $\partial K_{\tau_{m-1}}$ evaluated on ∂K_σ. In the form (5) the advantages of the formulation become rather clear, as it entails only discretizations of slow modulations and integrations that can be localized to the neighborhood of critical points; see [2, 5].

Enhanced Convergence by Analytic Continuation

As has recently been shown (see [2–4]), within the context of several interacting convex structures, the (spectral) convergence of the Neumann series is governed by the underlying geometrical configuration. More precisely, considering for simplicity the case of two cylindrical convex structures K_1 and K_2, the (high-frequency) rate of convergence of the Neumann series is given, asymptotically as $k \to \infty$, by

$$\mathcal{R}_k = e^{2ikd}\left(\sqrt{r} + \sqrt{r-1}\right)^{-1} \tag{6}$$

where $d = \operatorname{dist}(K_1, K_2)$, $r = (1 + d\kappa_1)(1 + d\kappa_2)$ and κ_j are the curvatures at the distance minimizing points. The spectral rate in (6) suggests that, as long as $r > 1$, the series can be interpreted as a power series in an artificial parameter z evaluated at $z = 1$. At high-frequencies, the radius of convergence of this series will thus be limited (it will approach R_k^{-1}) but its convergence can be enhanced via classical Padé approximation; see [5].

A New Krylov-subspace Based Acceleration Strategy

Although, as shown in [5] (see also Figure 1), the use of Padé approximation significantly accelerates the convergence of multiple scattering iterations, it is not optimal from this perspective. In the present context, a most relevant property of the Padé approximants relates to the possibility of evaluating these from the sole knowledge of the iterates $T^m g$, whose calculation can be done in frequency independent times. Indeed, the new high-frequency integral equation approach allows for the efficient evaluation of the Krylov subspace associated with the operator T or, equivalently, that of $I - T$. And this, in turn, suggests that a best approximation to the solution of equation (3) can alternatively be garnered through the application of optimized Krylov subspace methods (e.g. GMRES).

In more detail, and letting $A = I - T$, a basis $p_0, p_1, \ldots, p_{m-1}$ for the Krylov subspace

$$\mathcal{K}_m(A, g) = \operatorname{span}\{g, Ag, \ldots, A^{m-1}g\}$$

can be effectively computed through the classical recursion

$$p_{j+1} = A\,p_j + \sum_{i=0}^{j} \beta_{ij}\,p_i \tag{7}$$

provided efficient evaluations of $A^m g$ can be attained. Clearly, a most natural approach would rely on the *binomial theorem*

$$A^m = \sum_{j=0}^{m} \binom{m}{j} (-1)^j\, T^j \tag{8}$$

as this reduces the problem to the fast evaluation of the iterates $T^j g$ entering the Neumann series. We note, however, that the convergence of this Krylov-subspace technique is strongly affected by the *direct* use of (8) as it impairs the approximation of each projection A^m (see Figure 1). On the other hand, owing to (8), we have

$$\mathcal{K}_m(A, g) = \mathrm{span}\{g, Tg, \ldots, T^{m-1}g\}\,,$$

and thus, the representation

$$p_j = \sum_{i=0}^{j} \gamma_{ij} T^i g \tag{9}$$

delivers the *stable* recursion (see [6])

$$\begin{aligned} p_{j+1} &= (I - T)p_j + \sum_{i=0}^{j} \beta_{ij} p_i \qquad (10)\\ &= \sum_{i=0}^{j} \gamma_{ij} T^i g + \sum_{i=0}^{j} \gamma_{ij} T^{i+1} g + \sum_{i=0}^{j} \beta_{ij} p_i \end{aligned}$$

replacing the combined use of (7) and (8).

Numerical Example

In Figure 1, we present a comparison of (a) the Neumann series; (b) the Padé approximation; (c) a Krylov subspace method (GMRES) based on the binomial formula (8); and (d) the alternative implementation of the latter based on the decomposition (9) leading to equation (10). Here we have considered the configuration in Figure 1 (top) consisting of two elliptical cylinders with centers at $(0, 0)$ and $(0, -4.5)$, and major/minor axes $10/1$ and $7/2$. The illumination is provided by a plane wave with direction along the major axes and wavenumber $k = 40$. The bottom figure displays the number of reflections versus the relative L^∞ error between the exact solution and the approximations obtained by the four aforementioned schemes.

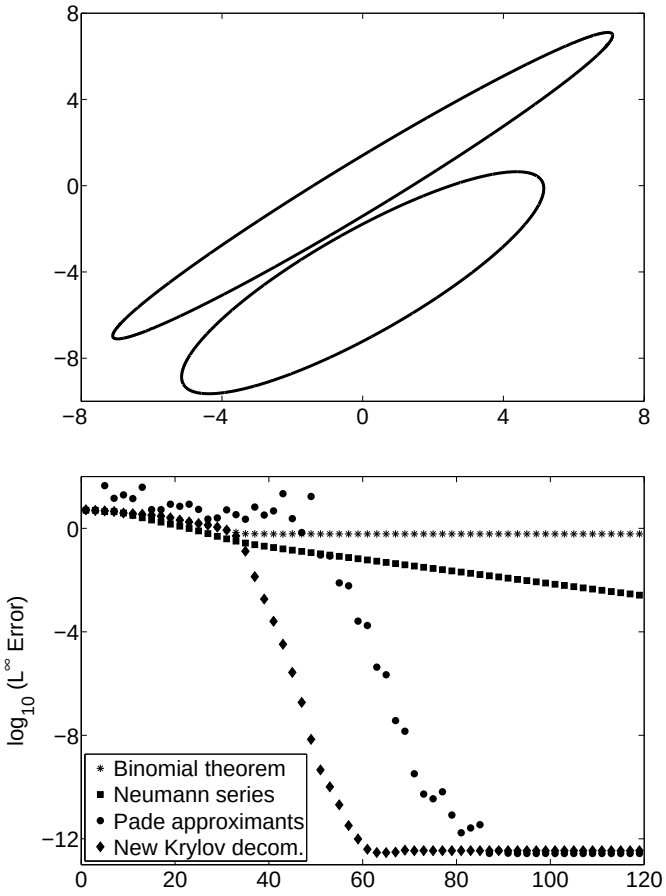

Figure 1: Top: A configuration with two ellipses. Bottom: Number of reflections vs. logarithmic plot of L^∞ error.

References

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