NOTE

Efficient Implementation of the Exact Numerical Far Field Boundary Condition for Poisson Equation on an Infinite Domain

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I. INTRODUCTION

Computation of exterior fluid problems often involves solving the Poisson equation in an unbounded domain. To cut down computational cost, it is desirable to minimize the computational domain. Therefore an important numerical issue is how to specify correctly the boundary condition at a finite computational boundary. In this note, we present an efficient method for such a task.

The basic idea behind the current work and many previous works (see, for example, [1–4]) exploits solutions to the Laplace equation outside the compact support of the source. Therefore, in theory, all these methods are equivalent. However, the current numerical implementation is simpler than that of previous methods. In particular, we solve the Poisson equation with a false Dirichlet boundary condition, from which the correct solution can be obtained. This avoids handling mixed boundary conditions in the far field such as those used by Keller and Givolli [1]. Moreover, our strategy is independent of the discretization scheme; thus the derivation is more transparent than derivations employing explicit differencing schemes, as in the work of Anderson and Reider [3]. Because our method is independent of the discretization scheme, it can be implemented straightforwardly using a variety of discretization schemes, including finite difference and finite element methods. The current method can also be more efficient in high-order schemes than other methods involving inverting matrices whose complexity depends on the order of finite differencing [4]. Finally,

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it does not require the explicit form of the correct far field boundary condition; thus we sidestep the Gaussian elimination procedure in the method of Anderson and Reider [3].

II. METHOD

We will restrict our attention to the two dimensional Poisson equation whose source has a compact support, and will derive the general scheme for a Poisson problem outside a cylinder. We remark that the same scheme applies, after a transformation, to all other conformal geometries such as an ellipse or a Joukowski airfoil.

Let \( R_1 \) be the radius of the cylinder, \( R_2 \) the radius of the computational boundary, and \( a \) the radius of the compact support of the source term; they satisfy the relation \( R_1 < a < R_2 \).

We need to numerically solve the Poisson equation,

\[
\Delta \Psi(r, \theta) = \omega(r, \theta),
\]

with known boundary condition at \( R_1 \). In theory, the exact solution can be obtained by convolving the source term with the Green function of the exterior problem. However, straightforward numerical integrations are expensive unless one resorts to special methods such as the fast multipole methods [5]. Alternatively and more conventionally, one solves Eq. (1) in an annulus between \( R_1 \) and \( R_2 \) by methods using Fast Fourier Transforms (FFT). This then requires the specification of the boundary condition at the computational boundary \( R_2 \), in addition to the physical boundary condition at \( R_1 \). In our approach we circumvent the problem by first solving the Poisson equation with a false boundary condition at \( R_2 \), and then extracting the correct solution from it.

Let \( \tilde{\Psi}(r, \theta) \) be the false solution, which satisfies Eq. (1) with boundary conditions

\[
\tilde{\Psi}(R_1) = \Psi(R_1),
\]

\[
\tilde{\Psi}(R_2) = \Gamma \ln(R_2),
\]

where \( \Gamma \) is the total circulation. Our aim is to obtain \( \Psi(r, \theta) \) from \( \tilde{\Psi}(r, \theta) \) by subtracting the error \( \Psi_1(r, \theta) \), which satisfies the Laplace equation, \( \Delta \Psi_1(r, \theta) = 0 \), and has a formal solution,

\[
\Psi_1(r, \theta) = \Gamma_1 \ln r + \sum_{n \geq 1} \left( B_n r^n + \frac{C_n}{r^n} \right) e^{i n \theta}, \quad R_1 < r < R_2,
\]

where the unknown constants \( \Gamma_1, B_n \), and \( C_n \) can be determined from the boundary conditions, Eqs. (2), (3), together with the radial derivative of \( \tilde{\Psi}(r, \theta) \) at \( R_2 \), which is harmonic. This follows from the fact that \( \Psi \) outside the compact support is harmonic and has a solution

\[
\Psi(r, \theta) = \Gamma \ln r + \sum_{n \geq 1} A_n \frac{e^{i n \theta}}{r^n} \quad \text{for } r > a.
\]

Using Eqs. (4) and (5), we obtain

\[
\frac{\partial \tilde{\Psi}}{\partial r}(r, \theta) = \sum_{n \geq 1} n B_n r^{n-1} e^{i n \theta} - \sum_{n \geq 1} n \left( A_n + C_n \right) \frac{e^{i n \theta}}{r^{n+1}} + \frac{\Gamma + \Gamma_1}{r}, \quad \text{for } r > a.
\]
The left-hand side is known and we denote its Fourier coefficients as $f_n$,
\[ \frac{\partial \Psi}{\partial r}(r, \theta) \equiv f_0 + \sum_{n \geq 1} f_n(r)e^{in\theta}. \] (7)

Using Eqs. (2), (3), (6) we can express $A_n$, $B_n$, and $C_n$ in terms of $f_n$,
\[ \Gamma_1 = 0, \] (8)
\[ A_n = (R_1^{2n} - R_2^{2n})B_n, \] (9)
\[ B_n = \frac{f_n}{2nR_2^{n-1}}, \] (10)
\[ C_n = -B_nR_1^{2n}. \] (11)

Consequently, the correct solution $\Psi(r, \theta)$ is given by
\[ \Psi(r, \theta) = \tilde{\Psi}(r, \theta) + \sum_{n \geq 1} \frac{f_n(R_2)}{2nR_2^{n-1}} \left( r^n - \frac{R_1^{2n}}{r^n} \right) e^{in\theta}. \] (12)

$f_n(R_2)$ and the sum in the last equation can be evaluated via FFT.

III. NUMERICAL IMPLEMENTATIONS AND RESULTS

In this section we illustrate the method by considering a simple example,
\[ \Delta \Psi = \frac{r(1 + r)\cos \theta + (3 + r)\sin 2\theta}{r^3}e^{-r}, \] (13)
which has the exact solution
\[ \Psi_e = \frac{1 + e^{-r}}{r} \cos \theta + \frac{1 + e^{-r}}{r^2} \sin 2\theta. \] (14)

Note that the source term in Eq. (13) decays exponentially in $r$; thus the potential solution gives a good approximation in the far field.

To take advantage of FFT in solving Eq. (13), it is convenient to transform the cylindrical coordinates to a uniform grid by defining a new variable $\mu = \ln(r)$. In the new coordinates $(\mu, \theta)$, we have
\[ \frac{\partial^2 \Psi(\mu, \theta)}{\partial^2 \mu} + \frac{\partial^2 \Psi(\mu, \theta)}{\partial^2 \theta} = e^{2\mu} \omega(\mu, \theta), \quad \theta \in [0, 2\pi], \mu \in [\mu_1, \mu_2]. \] (15)

where $\omega(\mu, \theta)$ corresponds to the right-hand side of Eq. (13). Following the procedure described in the previous section, we first solve $\Psi$ using a false boundary condition at $\mu_2$ in addition to the known boundary condition at $\mu_1$; $\tilde{\Psi}|_{\mu_1} = \Psi_e(\mu_1, \theta)$ and $\tilde{\Psi}|_{\mu_2} = 0$. The solution is then corrected by Eq. (12), with $r$ a function of $\mu$.

In this example, the computational domain is specified by parameters $\mu_1 = 2$ and $\mu_2 = 3$. In Figs. 1a and 1c, we plot the solutions at a given radius along the azimuthal direction. We compare the exact solution, the solution with a false boundary condition, and the corrected solution near the far field boundary, $r = R_2 - dr$, and in the middle of the computational domain, $r = R_2/2$.

Since the corrected solution satisfies the far field boundary condition exactly in theory, the numerical accuracy is only limited by the discretization scheme. In this example, because
FIG. 1. (a) Comparison among the exact solution, $\Psi_e$, the numerical solution with the false boundary condition, $\Psi_f$, and the corrected solution, $\Psi_c$, as a function of the azimuthal angle, which is labeled by the discrete index $j$. $r = R_2 - 2dr$, and the grid size is $32 \times 32$. (b) Convergence test using three different resolutions: $32 \times 32$, $64 \times 64$, and $128 \times 128$. The vertical variable corresponds to $(\Psi - \Psi_c)/dr^2$. Figures 1c and 1d are the same as Figs. 1a and 1b, respectively, except that $r = R_j/2$.

FIG. 2. Comparison of the normalized errors shown in Fig. 1d (circles) and those due to pure discretization (line). The latter is obtained by numerically solving the Poisson equation with the exact analytic boundary condition specified by Eq. (14).
we use center differencing at the boundary points, the numerical accuracy is of second order. This is checked by comparing the solutions using three different grid sizes: 32 $\times$ 32, 64 $\times$ 64, and 128 $\times$ 128. In Figs. 1b and 1d, we show the convergence of the errors normalized by $dr^2$. We can further show that the spatial variation of these errors arises mostly from the discretization procedure. To illustrate this, we compute the numerical solution with the exact boundary condition given by the analytic expression in Eq. (14). The numerical errors in this case are only due to discretization and round-off errors. Next we compare these errors with those shown previously in Fig. 1d. The difference is rather small, as can be seen in Fig. 2. The small difference can be attributed to the source term excluded from the computational domain, and the errors introduced by the procedure for correcting the solution are insignificant. Finally, the requirement of the compact support of the source term may not be satisfied exactly in practice. Nonetheless, one can estimate this type of errors using the multipole moments of the excluded source. These estimates then determine an appropriate size of the computational domain for a target accuracy.

IV. CONCLUSION

In conclusion, the correct solution to the Poisson equation in an unbounded domain can be obtained without specifying explicitly the correct far field boundary condition. A false solution with a Dirichlet boundary condition is “self-correctable,” because the error everywhere in the domain is completely determined by the behavior of the false solution at far field, whose form is known analytically. Computationally, the correction is straightforward with essentially an additional FFT. Although our example employs a finite differencing scheme, our general method can be readily implemented using other discretization schemes. The current scheme should be useful in the computation of fluid problems such as flow past a cylinder or other conformal geometry, where the Poisson solver is usually the workhorse. Finally, the “self-correction” strategy explored here should be applicable to Poisson equations in high dimensions as well as other linear equations such as the Helmholtz equation, where the harmonic series are replaced by appropriate eigenfunctions.

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