Highly Accurate Implementations of Methods for Handling Singularities on a Planar Patch

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Abstract **–** Three methods for evaluating integrals containing the Green's function singularity are studied from the standpoint of numerical accuracy at levels required in high order calculations. A significant source of potential error was found to be common to all methods. Suggestions for improving the accuracy of all three are proposed.

Keywords: Green's function singularity, singularity extraction, Duffy transformation, arcsinh transformation, integral equation, method of moments, high order, and boundary element method.

I. INTRODUCTION

In a recent paper [1], the authors developed an exact-to-machine-precision method for the evaluation of the free-space Green's function on a rectangular patch. This result was then used to examine the singularity extraction and singularity cancellation methods as a function of the ratio of the sides of a rectangular patch, using the corresponding exact result for comparison. It was found that the aspect ratio of the patch, and the triangles contained therein, had a significant effect on the accuracy associated with the schemes studied. In order to overcome the accuracy problems identified, a number of remedies were proposed. These remedies mainly involved using higher precision in the calculations, making them unattractive to potential users. Since paper [1] was published, a paper by Khayat and Wilton introduced a new singularity cancellation method using an arcsinh transformation [2], possibly overcoming the drawbacks of the remedies just referred to. Here we examine the arcsinh method in comparison to the two methods, already studied, and augment the conclusions of the previous paper. In addition, we identify one of the principal causes of error in our implementation of the three methods.

The objectives here are to: 1) examine the arcsinh method and compare it with the earlier results, 2) explain the cause of the inaccuracies found in all three methods and 3) test all three methods over the widest range of the aspect ratio of the patch that may be encountered in practice.

The range of aspect ratios is determined by consideration of test point locations on a patch. In practice, the domain of a patch is divided into four rectangular sub-patches each with a corner at the test point. The location of the test point, and hence the aspect ratio of each sub-patch, is controlled by the quadrature rule employed to perform the required integrations. As shown in [1], this can lead to a sub-patch aspect ratio up to 1:10^{-10}. This observation determines the range of aspect ratios over which the tests are performed. The ratio may seem extreme, but the primary motivation for this work is to obtain accuracy near the limit of machine precision, which is an important requirement in high order numerical solutions of integral equations.

II. REVIEW OF METHODS

The integral to be evaluated has the form,

$$I(x,y) = \iint f(x',y') \frac{e^{-jkR}}{R} dx'dy' \qquad (1)$$

where f is usually a bounded, well-behaved function, $k = 2\pi/\lambda$ where λ is the wavelength, and R is given by,

$$R = \sqrt{(x-x')^2 + (y-y')^2} \qquad (2)$$

The accurate evaluation of equation (1) is most difficult when the test point (x,y) is within or near the source cell over which the integral is performed, due to the O(1/R) behavior of the Green's function, e^{-jkR}/R.

In the earlier paper [1], we examined the singularity extraction, SE, procedure and the Duffy transformation [3]. These methods are fully described in that paper. A third approach for evaluating equation (1) is the *arcsinh transformation* proposed by Khayat and Wilton [2] which is described next. For a rectangular domain $0 < x' < a$, $0 < y' < b$ and the test point at x=y=0, the domain is divided into triangles along the line $y' = b/a\ x'$. We introduce the change of variable indicated in equation (3) in the first integral and the substitution of equation (4) in the second integral. This leads to equation (5) or, equivalently, (6). The integrands in equation (6) are bounded and amenable to numerical quadrature.

For a number of specific functions *f*, including *f(x,y)*=1, one of the integrals in each of the double integrals arising from the Duffy and the arcsinh approaches can be performed analytically. To ensure a fair comparison with the SE procedure, we do not take advantage of that step in the following, although in practice it would make sense to do so.

III. METHODOLOGY

The present study investigates the numerical accuracy obtained from the preceding methods, using single and double precision for some or all of the calculations, for the case *f(x,y)*=1. Many bounded functions could be used for *f(x,y)*. The procedure used to determine the reference values requires that a function of the form *f(x,y)*= x^m y^m, where $0 \le n,m$, be used. However, a constant *f(x,y)* is considered sufficiently challenging. The domain of integration is a patch that has one side of dimension 0.1λ and the other of dimension 10^{-n} λ, where $1 \le n \le 11$. The test point is at one corner. As discussed in [1] it is instructive to examine a wide range of cell aspect ratios, and we consider K ranging from $1{:}1$ to 10^{-10} :1. This is particularly important when using high order basis functions and/or over-determined systems where many test points are present on the patch. As a baseline for comparison, a reference result for equation (1) was obtained using the approach of [1]. The reference was evaluated in Multi-Precision arithmetic [4] using an epsilon value of 10.0^{-400}. The reference values are shown in Table 1 to double precision accuracy.

$$y' = x' \sinh u, \quad dy' = x' \cosh u du$$
$$= x' \sqrt{1+\left(\frac{y'}{x'}\right)^2} du = \sqrt{x'^2 + y'^2} du = R du \tag{3}$$

$$\begin{gathered} x' = y' \sinh v, \\ dx' = y' \cosh v \, dv = \sqrt{y'^2 + x'^2} dv = R dv \end{gathered} , \tag{4}$$

$$\begin{aligned} I(x,y) = & \int_{x'=0}^{a} \int_{u=0}^{\sinh^{-1}(K)} f\left(x', x'\sinh(u)\right) e^{-jkR} du dx' \\ & + \int_{y'=0}^{b} \int_{v=0}^{\sinh^{-1}(1/K)} f\left(y'\sinh(v), y'\right) e^{-jkR} dv dy' \end{aligned} , \tag{5}$$

$$\begin{aligned} I(x,y) = & \int_{x'=0}^{a} \int_{u=0}^{\sinh^{-1}(K)} f\left(x', x'\sinh(u)\right) e^{-jkx'\cosh(u)} du dx' \\ & + \int_{y'=0}^{b} \int_{v=0}^{\sinh^{-1}(1/K)} f\left(y'\sinh(v), y'\right) e^{-jky'\cosh(v)} dv dy' \end{aligned} . \tag{6}$$

Table 1. Values for the value of the integral defined in equation (1) for the range of aspect ratios used in this study.

Aspect Ratio	Real	Imaginary
1	1.615721995380920E-01	-6.012599373499612E-02
0.1	3.898233302555344E-02	-6.145640913466086E-03
1.00E-02	6.201218961036034E-03	-6.146987225913048E-04
1.00E-03	8.503815540084963E-04	-6.147000690637945E-05
1.00E-04	1.080640082293225E-04	-6.147000825285354E-06
1.00E-05	1.310898591857477E-05	-6.147000826631829E-07
1.00E-06	1.541157101160280E-06	-6.147000826645292E-08
1.00E-07	1.771415610459726E-07	-6.147000826645428E-09
1.00E-08	2.001674119759131E-08	-6.147000826645429E-10
1.00E-09	2.231932629058536E-09	-6.147000826645429E-11
1.00E-10	2.462191138357940E-10	-6.147000826645429E-12

The double integrals examined here were evaluated using the product of adaptive Gauss-Kronrod-Patterson quadrature rules [5], starting with 15 nodes and proceeding to 511 nodes if/when needed. The integration cycle was terminated when two consecutive values differed by less than 2ε (where ε is the operating precision).

The different singularity-handling schemes were evaluated using the relative error.

$$Error = \log_{10} \left| \frac{I - I_{ref}}{I_{ref}} \right| . \tag{7}$$

Here, I and I_{ref} are the values of the relevant integral and the reference value, respectively, evaluated in the stated machine precision. The smallest error is limited by the precision of the compiler used for the calculations. Here those limits are -6.92360 and -15.6536 for single and double precision, respectively.

The work reported here was conducted using Fortran90. The available compiler did not include the inverse hyperbolic functions. Consequently $\sinh^{-1}$(K) was initially calculated using the widely accepted definition [6, p178],

$$\sinh^{-1}(x) = \ln\left(x + \sqrt{x^2+1}\right) . \tag{8}$$

IV. RESULTS

When the above singularity removal methods are evaluated in the various machine precisions, for $f(x,y)=1$, the findings in Tables 2 and 3 are obtained (the relevant results for SE and Duffy from the earlier study are reported here for ease of comparison purposes). The results indicate that all methods degrade in accuracy as the cell aspect ratio increases. Tables 2 and 3 report error in the real part of the integral. For the imaginary part, both the SE and Duffy methods maintain accuracy over the entire range tested. On the other hand, the arcsinh method showed deterioration in the imaginary part that is similar to that observed in Tables 2 and 3 in the real part as the aspect ratio is decreased.

Table 2. Relative error in the real part of equation (1) when using single precision.

	Singularity Removal Method.		
Aspect Ratio	SE	Duffy	Arcsinh
1	-6.92369	-6.92369	-6.92369
0.1	-6.41765	-6.92369	-6.92369
1.00E-02	-5.94832	-6.92369	-6.04523
1.00E-03	-5.07121	-6.92369	-5.57357
1.00E-04	-3.90065	-4.09225	-4.95281
1.00E-05	-2.42700	-2.08886	-4.01513
1.00E-06	2.73E-03	-1.10230	-2.55098
1.00E-07	2.37E-03	-0.70402	-1.99378
1.00E-08	2.10E-03	-0.53765	-1.33035
1.00E-09	1.89E-03	-0.43983	-1.37764
1.00E-10	1.71E-03	-0.37390	-1.42028

Table 3. Relative error in the real part of equation (1) when using double precision.

	Singularity Removal Method.		
Aspect Ratio	SE	Duffy	Arcsinh
1	-15.6536	-15.6536	-15.6536
0.1	-15.6536	-15.6536	-15.6536
1.00E-02	-14.1219	-15.6536	-14.9000
1.00E-03	-13.5385	-15.6536	-14.2413
1.00E-04	-12.2983	-11.2123	-13.6050
1.00E-05	-11.7914	-5.33437	-12.3036
1.00E-06	-10.1758	-3.62397	-11.6391
1.00E-07	-9.18065	-1.50125	-10.5242
1.00E-08	-8.38368	-0.85638	-9.28591
1.00E-09	-8.43096	-0.64213	-8.46256
1.00E-10	-6.14382	-0.52264	-8.50283

V. DISCUSSION

It was observed in [1] that the performance of the SE method can be improved to full precision if the extracted term is evaluated at the next higher precision level. It was also pointed out that the Duffy method could be similarly improved if the SE procedure was applied to the integrals involved in the Duffy procedure. This results in two bounded integrals and two extracted terms. For the improved Duffy method, the extracted term must also be evaluated in the next higher precision [1]. In this study, we also found that the arcsinh method can be improved by employing the next higher precision for the evaluation of the integration limit, $\sinh^{-1}(K)$ using equation (8).

A review of these remedies for the SE and improved Duffy methods revealed that the need for higher precision arose in connection with those extracted terms that have the same form as equation (8) for $\sinh^{-1}(K)$, namely $\log\left(K+\sqrt{K^2+1}\right)$ [6, p. 420]. Further investigation, involving the use of three different commercial Fortran90 compilers, revealed that there is significant rounding/truncation error in the evaluation of that function for small K. (Compilers that provide an intrinsic function for $\sinh^{-1}(K)$ worked correctly.) As an alternative to the use of higher precision as recommended in [1], we employed the Newton-Raphson procedure [6, p. 355] to evaluate the function $\log\left(K+\sqrt{K^2+1}\right)$ by solving for x in,

$$f=\sinh(x)-K=0 \; . \qquad (9)$$

The Newton-Raphson procedure was terminated when two consecutive values differed by less than 2ε (where ε is the operating precision). A code fragment for the evaluation of $\sinh^{-1}(K)$ is provided in Figure 1. When $\sinh^{-1}(K)$ in the arcsinh formulation, and $\log\left(K+\sqrt{K^2+1}\right)$ in the SE and improved Duffy procedures, was evaluated using the Newton-Raphson approach, the results shown in Tables 4 and 5 were obtained.

When the Newton-Raphson method is used to evaluate $\sinh^{-1}(K)$, or $\log\left(K+\sqrt{K^2+1}\right)$, in the various methods, both the real and imaginary parts of equation (1) retain essentially full precision for all three approaches.

The procedures necessary to maintain essentially full precision with the three different methods when integrating the Green's function are summarized in Table 6.

Table 4. Relative error in the real part of equation (1) when using single precision and the Newton-Raphson method.

	Singularity Removal Method.			
Aspect Ratio	SE	Duffy	Improved Duffy	Arcsinh
1	-6.92369	-6.92369	-6.92369	-6.92369
0.1	-6.92369	-6.92369	-6.92369	-6.92369
1.00E-02	-6.92369	-6.92369	-6.92369	-6.92369
1.00E-03	-6.92369	-6.92369	-6.92369	-6.92369
1.00E-04	-6.92369	-4.09225	-6.92369	-6.87076
1.00E-05	-6.92369	-2.08886	-6.92369	-6.92369
1.00E-06	-6.92369	-1.10230	-6.92369	-6.92369
1.00E-07	-6.92369	-0.70402	-6.92369	-6.92369
1.00E-08	-6.92369	-0.53765	-6.92369	-6.92369
1.00E-09	-6.92369	-0.43983	-6.92369	-6.92369
1.00E-10	-6.92369	-0.37390	-6.92369	-6.92369

Table 5. Relative error in the real part of equation (1) when using double precision and the Newton-Raphson method.

	Singularity Removal Method.			
Aspect Ratio	SE	Duffy	Improved Duffy	Arcsinh
1	-15.6536	-15.6536	-15.6536	-15.6536
0.1	-15.6536	-15.6536	-15.6536	-15.6536
1.00E-02	-15.6536	-15.6536	-15.6536	-15.6536
1.00E-03	-15.1955	-15.6536	-15.6536	-15.6006
1.00E-04	-14.4545	-11.2123	-15.6536	-15.6536
1.00E-05	-13.4821	-5.33437	-15.6536	-15.6536
1.00E-06	-14.3435	-3.62397	-15.6536	-15.6536
1.00E-07	-15.6536	-1.50125	-15.6536	-15.6536
1.00E-08	-15.6536	-0.85638	-15.6536	-15.6536
1.00E-09	-15.6536	-0.64213	-15.6536	-15.4311
1.00E-10	-15.6536	-0.52264	-15.6536	-15.6536

The integrals considered here are expressed in the Cartesian coordinate system. In a non-Cartesian system the above remedies still apply — so long as closed-form solutions for the extracted terms are available. The arcsinh method avoids this requirement, but does require that an invertible transformation be identified. In more general constructions where cells might be mapped to curved surfaces, and the integrand contains an additional Jacobian, the preceding observations may not apply.

Table 6. Summary of procedures for the high accuracy evaluation of equation (1).

Method	Approach
SE	▪ Must have closed-form integral for the extracted term ▪ $\log\left(K+\sqrt{K^2+1}\right)$ must be evaluated carefully, here by Newton-Raphson.
Duffy	▪ Only the improved form is viable over the whole range ▪ Singularity extraction needs to be applied to the two main integrals ▪ Must have closed-form integrals for the extracted terms ▪ $\log\left(K+\sqrt{K^2+1}\right)$ must be evaluated carefully, here by Newton-Raphson.
Arcsinh	▪ $\sinh^{-1}\left(K\right)$ must be evaluated carefully, here by Newton-Raphson.
Duffy	▪ Only the improved form is viable over the whole range ▪ Singularity extraction needs to be applied to the two main integrals ▪ Must have closed-form integrals for the extracted terms ▪ $\log\left(K+\sqrt{K^2+1}\right)$ must be evaluated carefully, here by Newton-Raphson.

```
Function asinh(x)
!  This program uses Newton-Raphson to calculate
arcsinh(x)
            implicit real*8 (a-h, o-z)
            d0=float(0)
            d1=float(1)
            d2=float(2)
            xlimit=d2*epsilon(d1)
!
            uold=d0
!  Select a starting point – this is somewhat arbitrary
            if(x .lt. d2) then
                        unew=sign(d1,x)
            else
                        unew=sign(d1,x)*log(abs(x))
            endif
            do while(abs(unew – uold) .gt. xlimit)
                        f=sinh(unew)
                        df=cosh(unew)
                        correction=(f – x)/df
                        uold=unew
                        unew=uold – correction
            end do
!
            asinh(x)=unew
return
```

Fig. 1. Fortran90 code for inverse hyperbolic sine function.

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