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Evaluation of oscillatory integrals for analytical groundwater flow and mass transport models

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ABSTRACT

Modeling of transient dynamics of an interface between fluids of identical density and viscosity, but different otherwise, is of great interest in aquifer hydraulic, and advective contaminant transport, and has broad application. Closed-form solutions are often available for problems with simple, practically important geometry, but the integrals that appear in such solutions often have integrands with two or more oscillatory factors. Such integrals pose difficulties for numerical evaluation because the positive and negative contributions of the integrand largely cancel and the integrands decay very slowly in the integration domain. Some problems with integrands with a single oscillatory factor were tackled in the past with an integration/summation/extrapolation (ISE) method: breaking the integrand at consecutive zeros to obtain an alternating series and then using the Shanks algorithm to accelerate convergence of the series. However, this technique is ineffective for problems with multiple oscillatory factors. We present a comprehensive strategy for evaluation of such integrals that includes a better ISE method, an interval truncation method, and long-time asymptotics; this strategy is applicable to a large class of integrals with either single or multiple oscillatory factors that arise in modeling of groundwater flow and transport. The effectiveness of this methodology is illustrated by examples of integrals used in well hydraulics, groundwater recharge design, and particle tracking.

1. Introduction

One problem of interest in hydrogeology is the dynamics of an interface between two fluids with similar density and viscosity, but with different water quality. An example is managed aquifer recharge, where two fluids may differ just by the presence of biological agents in tiny concentrations. In such cases, particle tracking is the most direct tool for modeling a moving interface with high resolution in time and space, spared of numerical dispersion effects, and is well suited for modern visualization tools. Many 3D problems of groundwater flow hydraulics have closed-form solutions consisting of integrals on an infinite domain with oscillatory factors in the integrands. In managed aquifer recharge and water quality studies, these are trigonometric functions in Cartesian coordinates (Zlotnik and Ledder, 1993) or Bessel functions in cylindrical coordinates (Bruggeman, 1999; Dagan, 1967; Hantush, 1967; Zlotnik and Ledder, 1992). Although the idea is straightforward, this approach requires a large number of computations of integrals that represent the hydraulic head and velocity; thus, any difficulty in integral computation hinders application of particle tracking algorithms. Such applications create a need for computationally efficient evaluation of integrals with oscillatory integrands. No one method is ideal for all cases, so the best practical approach is to devise a comprehensive strategy that balances the needs for high precision and reasonable computational time by blending sophisticated methods as needed with fast methods when possible.

In principle, one can use a standard quadrature method to integrate over an interval [0, U], where U is large enough for the error caused by the domain truncation to be small. (See Auluck, 2012, for example.) This is inefficient for integrands with slowly decaying amplitudes, such as products of two Bessel functions, because the positive and negative portions of the integrand largely cancel out, making the computation slow and susceptible to round-off errors. While this approach seems too naïve to be of value, it can be the method of choice for some problems, provided the amplitude decay is not too slow and a suitable upper bound value can be determined. We present a practical solution to this problem in the methods section.

The computation of integrals with oscillatory integrands has been addressed for some specific groundwater flow problems.

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Peng et al. (2002) obtained an integral for the hydraulic head in a confined aquifer with constant head at the wellbore:

$$h = 1 - \frac{2}{\pi}\int_0^\infty e^{-tu^2}\frac{J_0(u)Y_0(ru) - Y_0(u)J_0(ru)}{u[J_0^2(u)+Y_0^2(u)]}\,du. \tag{1}$$

To evaluate this integral, the integration domain was partitioned into segments between the zeros of the integrand. Gaussian quadrature was used to evaluate the integral on each segment, and then Shanks extrapolation was used to accelerate convergence of the sum.

Yeh et al. (2008) considered the drawdown resulting from a well with a constant pumping rate in a wedge-shaped region between two streams. The formula consists of an infinite sum over a discrete set of ν values of integrals of the form

$$\int_0^\infty \left(1 - e^{-tu^2}\right)u^{-1}J_\nu(ru)J_\nu(u)\,du. \tag{2}$$

The principal quantity of interest in this paper was the stream depletion rate, for which the integrals reduce to

$$\int_0^\infty \left(1 - e^{-tu^2}\right)u^{-1}J_\nu(u)\,du \tag{3}$$

by averaging over r. These authors computed the integrals (3) using the method of Peng et al. (2002), but they did not compute the integrals having two oscillatory factors (2).

Methods involving partition of an integral at regular intervals and summation of the approximations with a convergence accelerator are called ISE (Integration, Summation, Extrapolation) methods (see, for example, Davis and Rabinowitz, 1984). The ISE method used by Peng et al. is effective for their problem because the oscillatory function $J_0(u)Y_0(ru) - Y_0(u)J_0(ru)$ has zeros that become regularly spaced as $u \to \infty$. The same is true for (3); however, there are many important closed form groundwater flow formulas with multiple oscillatory integrand factors, such as (2). Other examples stem from infiltration at a uniform rate from a circular recharge basin, including the water table rise using the Dupuit–Forchheimer approximation (Hantush, 1967),

$$h^2 - h_0^2 = \frac{2V}{\pi K}f(q,\rho), \quad f(q,\rho) = \int_0^\infty \left(1 - e^{-qu}\right)J_0(\rho u)J_1(u)\frac{du}{u^2}, \tag{4}$$

the hydraulic head for a confined aquifer of infinite depth near a polder (Bruggeman, 1999),

$$h(r,z,t) = \frac{qR}{K}\int_0^\infty J_0(ru)J_1(Ru)P_c\left(\frac{uz}{2},\frac{u\sqrt{t}}{\beta}\right)\frac{du}{u}, \tag{5}$$

where

$$P_c(x,y) = \frac{1}{2}e^{2x}\mathrm{erfc}\left(\frac{x}{y}+y\right) - \frac{1}{2}e^{-2x}\mathrm{erfc}\left(\frac{x}{y}-y\right),$$

and the (dimensionless) hydraulic head in an unconfined aquifer (Zlotnik and Ledder, 1992),

$$h(r,z,t) = \int_0^\infty R\left(1 - e^{-tu\tanh u}\right)J_0(ru)J_1(Ru)\frac{\cosh zu}{u\sinh u}\,du. \tag{6}$$

In Section 2.2, we illustrate the failure of extrapolation methods when zeros of integrands are not evenly spaced.

Special methods have been developed for integrands that contain products of Bessel functions. Van Deun and Cools (2006), 2008) present methods for integrals of the forms

$$\int_0^\infty x^m\Pi_{i=1}^k[J_{\nu_i}(a_ix)]dx, \quad \int_0^\infty e^{-cx}x^m\Pi_{i=1}^k[J_{\nu_i}(a_ix)]dx,$$
$$\int_0^\infty \frac{x^m}{x^2+r^2}\Pi_{i=1}^k[J_{\nu_i}(a_ix)]dx, \tag{7}$$

but these can be used for groundwater flow only when there are no additional factors in the integrand.

A more general method is that of Lucas (1995), which applies to any convergent integral of the form

$$\int_0^\infty f(x)J_\mu(\rho x)J_\nu(\tau x)\,dx. \tag{8}$$

This method has found widespread application in other areas of science, but it appears to have been referenced only once for a groundwater flow application, and those authors did not actually use it for any computations (Tartakovsky et al., 2000). It has been extended and coded into a Matlab package (Ratnanather et al., 2014), which offers the possibility of a single method for all of the problems presented here. (At present there is no implementation of this algorithm in Mathematica.) This is a reasonable approach when computation time is unimportant, but we will see that considerable time can be saved by supplementing Lucas' method with more efficient ones.

Modern computer algorithms are designed to achieve almost unlimited precision, which is fine when the total number of computations is limited. However, there are circumstances where it is necessary to do a huge number of computations, and in these cases it is necessary to trade some precision for computational speed, particularly since groundwater flow models are just hydrogeological approximations and parameter values are not known to a high degree of accuracy. An example is a recharge management scenario, in which it may be important to track the progress of the interface between the resident water and the recharged water. This surface can be constructed from a set of particle paths, obtained by integrating the velocity vector over time from points on the initial interface. For the case of an aquifer of large horizontal extent with uniform circular areal recharge, the hydraulic head is given by (6) and the tracking procedure requires numerous computations of radial and vertical velocity integrals given in cylindrical coordinates (r, z) at time t by

$$V_r(r,z,t) = \int_0^\infty R\left(1 - e^{-tu\tanh u}\right)J_1(ru)J_1(Ru)\frac{\cosh zu}{\sinh u}\,du, \tag{9}$$

and

$$V_z(r,z,t) = -\int_0^\infty R\left(1 - e^{-tu\tanh u}\right)J_0(ru)J_1(Ru)\frac{\sinh zu}{\sinh u}\,du, \tag{10}$$

both for $r > 0$, $0 \le z \le 1$, $t > 0$, where R is the radius of the recharge basin. The total number of integral evaluations required to produce even a coarse movie of the surface is at least in the thousands and may be two orders of magnitude higher.

For a simulation that requires many thousands of integral computations, the total time requirement using Lucas' method is prohibitive, but there are other methods that are more efficient for some times and locations. The goal of this paper is to present a comprehensive strategy for combining a variety of methods for a broad class of problems that includes (2–6, 9, 10). The methods needed for this strategy are presented in Section 2 and applied to specific examples in Section 3 with a focus on comparison.

2. Methods

Models for axisymmetric groundwater flow in a region of infinite horizontal extent yield solutions that can be written generically as

$$I(r,z,t;\Psi,f,\phi) = \int_0^\infty \left(1 - e^{-t\phi(u)}\right)\Psi(u,r)f(u,z)\,du,$$
$$r,z,t \ge 0, \tag{11}$$

where r, z, and t are dimensionless radial and vertical coordinates and time; Ψ, f, and ϕ are given functions, with Ψ consisting of one or two bounded oscillatory factors and ϕ nonnegative and