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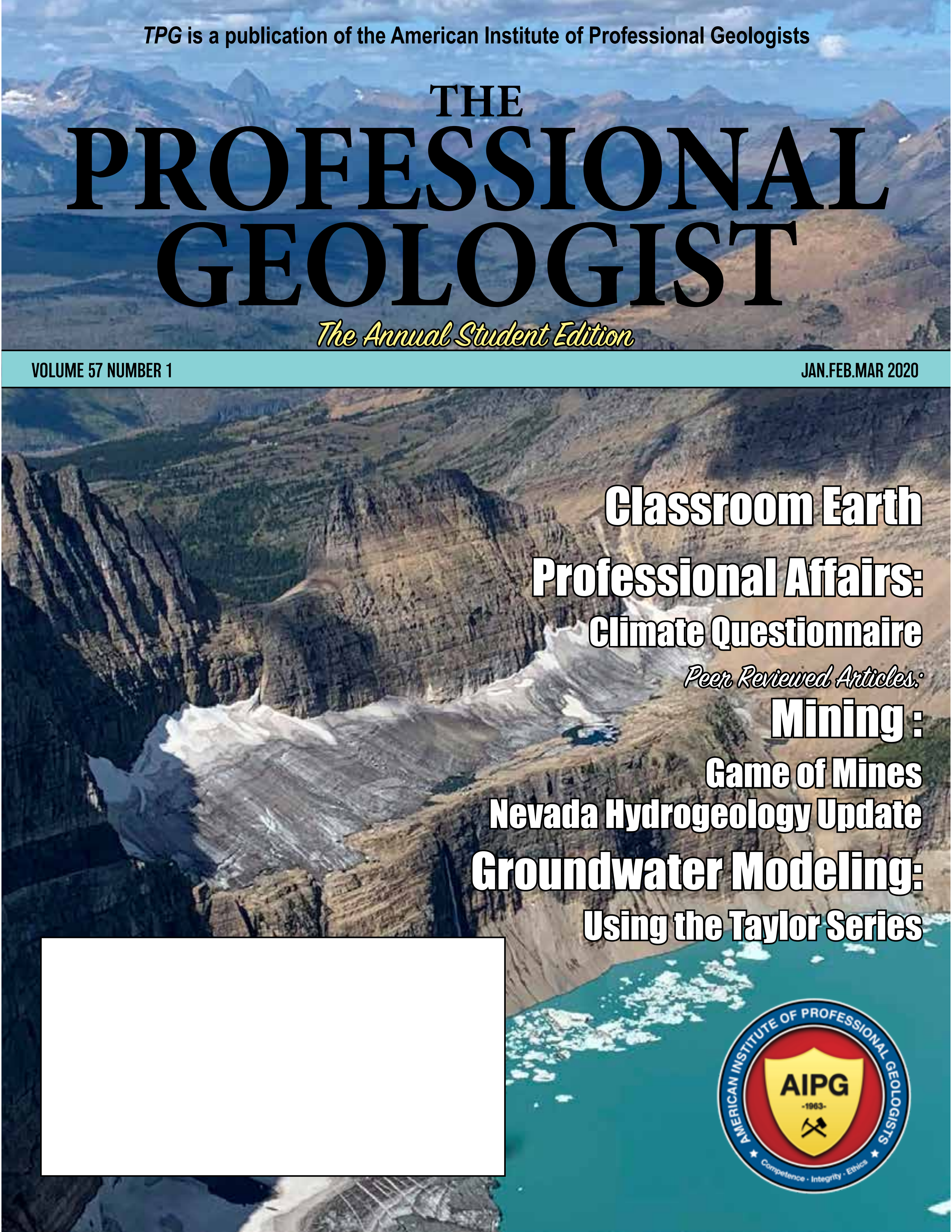

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Using Taylor Series to Assess Goodness of Groundwater Models



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Abstract

A problem of high interest to practitioners and researchers of groundwater flow problems is the goodness of outcomes produced from computational models. With domain-type computational models in frequent use - for example, those involving finite element, finite difference, finite volume, or other techniques - the topic of discretization effects is of high interest in assessing the goodness in model results. In this paper, we investigate the use of Taylor Series approximation to demonstrate the anticipated effectiveness of levels of discretization. We show how Taylor Series can be effectively used to evaluate anticipated departure between computational outcomes and the underlying analytic solution to the governing mathematical system of equations.

Keywords - Taylor Series, Groundwater Models, Complex Variable Boundary Element Method

Introduction

The Complex Variable Boundary Element Method (CVBEM) motivated this work by way of using approximations to solve complex variable equations, such as a complex variable Taylor Series. The CVBEM was introduced in Hromadka and Guymon (1984) and has been the subject of numerous investigations and applications throughout several facets of engineering. Among common applications of the CVBEM in engineering are fluid flow, hydraulics, and heat transfer. In 2002, Hromadka extended the CVBEM to three-dimensional (3D) domains of irregular geometry to accommodate practical problems that commonly occur in geoscience topics. For example, a 2017 study examines unsteady groundwater mounding problems (Wilkins, et al.) and Johnson et al. (2016) studied application in freezing and thawing soils in algid climates. Other applications are reported in the literature. More recently, Hromadka and Whitley (2014) provided a development of multi-dimensional applications using two-dimensional complex variable basis functions within the usual CVBEM framework. In tandem with this on-going research is the evolution of the visual computational error measure called the Approximate Boundary Method (ABM). First introduced in "CVBEM Error Reduction Using the Approximate Boundary Method" (Wood et al., 1993), the new techniques discussed here refine the accuracy achieved by the ABM by visually displaying the computational errors in position versus the number of nodes used in the approximation.

The CVBEM encompasses considerations of other variants of the general procedure such as the Method of Fundamental Solutions, or Generalized Fourier Series, and so forth. It is noted that the CVBEM is based upon use of complex variable analytic functions as basis functions.[1] Since the modeling basis functions are analytic, linear combinations are also analytic functions on a properly defined, simply connected domain, *D*, enclosed by a simple closed boundary, *B*. A real function that satisfies the Laplace equation is said to be "harmonic", and there exists an analytic function whose real part is the considered harmonic function. The Cauchy-Riemann equations state that the imaginary function portion of an analytic function is known within an integration constant, and can be determined from the real part of the analytic function. Therefore, both real and imaginary parts of the analytic function satisfy the Laplace equation and are harmonic functions. Additionally, being conjugate functions, level curves of the real part are orthogonal to level curves of the imaginary part, resulting in the well-known graphical display of "flow nets" that apply to numerous applications in science, mathematics, engineering and related fields. Such properties do not similarly exist for real value approximation functions and associated computational methods.

A Taylor Series expansion is a method used to evaluate a given function with infinitely many terms, as shown below. In engineering, these expansions are typically used to approximate functions by using only a small number of terms for a value when used to evaluate the function, ultimately saving time and resources for near-exact solutions. The successive derivatives, one of the unique features of a Taylor Series, are seen in the numerator of each term of the expression. In the complex domain, any function that is analytic at a given point, say z, will have a Taylor Series about that point. Therefore, it follows that the series will converge on $f(z)$ at each point z in

1. For discussion of a particular (but very important) case, see https://en.wikipedia.org/wiki/Basis_(linear_algebra)

the finite plane. Whenever a finite number of terms is used, it is considered a Taylor Series approximation. Several studies, including this one, focus on how efficient these approximations are for evaluating specific problems. The general case for the Taylor Series is

$$\mathrm{f}(z) = \sum_{n=0}^{\infty} \frac{f^n(z_0)}{n!}(z - z_0)^n$$

In this work, the CVBEM approximation technique will be formulated using complex polynomial (monomials) basis functions instead of the usual products of complex polynomials with complex logarithmic functions. The resulting formulation has direct ties with the Taylor Series formulation for analytic functions. Using flow nets developed from the CVBEM approximations, the modeling effort focuses on increasing computational accuracy until the CVBEM model flow net arrives at an acceptable geometric approximation to the problem boundary conditions. At this stage of model development, Taylor Series can be used to examine the precision of computations based upon the more general finite-difference, finite element, and finite volume type approaches. In this way, one can assess the precision of the domain model under consideration, and evaluate the departure between the domain model computational outcome and the underlying solution to the governing mathematical system of equations. Such assessment provides more information useful towards discretization density determination of modeling nodes and cells while possibly reducing computational burden.

Real Variable Taylor Series Animations

The Taylor Series corresponding to a function requires that the target function have derivatives of all orders. This requirement is similarly found with complex variable functions that are analytic. Both the real variable version and the complex variable version of Taylor Series are of similar construction, resulting in a sequence of function terms that relate the various orders of derivatives with monomial terms and associated constant coefficients. This sequence of terms is summed to form a series, where the first n terms is called the nth partial sum. Because the Taylor Series involves an infinite number of terms, only the initial portion of the series is used in approximation problems. How these "partial sums" behave is demonstrated by the example case studies presented and corresponding graphics. Intuitively, increases in the partial sum number of terms generally correspond to improved computational accuracy. Of special note is that the Taylor Series includes an error bound term that provides an upper bound estimate to computational error associated with a target partial sum. Of value to the computational modeling is that Taylor Series can be used as a case study to test the desired computational model and then use the resulting Taylor Series solutions and computational error for the known problem solution to assess the computational error associated with the target computational model as applied to the test problem. In this way, the Taylor Series can be used as a test case to assess the goodness of the target computational model, including issues such as modeling nodal point spacing and density, and so forth.

The sensitivity of the approximation to the number of terms, n, is demonstrated by the animations provided below. In the key to each graph, the numerical value is representative of the number of terms used in the evaluation. For instance, T0 is simply the function solved with $n = 0$, where T10 is the Taylor Series expansion to the 10th term. Figure 1 demonstrates the effectiveness of a partial sum on a function with a singularity at point $x = 1$.

In the following two figures, pay special attention to the fit of each line in respect to how many terms the line represents. Notice how the T0 is simply a line that only fits the specific value, and with the addition of each term the line becomes more closely related to the desired function. The T10 line stays along the original function line for the largest range of values, as anticipated.

In Figure 2, an example without a singularity, the difference is far more distinguished. Just as before, notice how the addition of terms makes the partial sum approximation more closely resemble the desired function.

Examining the Complex Variable Taylor Series Term

In the complex domain, a Taylor Series is a sum of complex monomials. Each complex monomial is an analytic function and is composed of its real part and corresponding imaginary part, with both parts being harmonic, two-dimensional real functions that satisfy the Laplace equation. Furthermore, these two parts satisfy the Cauchy-Riemann equations and therefore are complex conjugate functions where either part is derivable from the other. These can be visualized using flow nets. To demonstrate the flow nets for such complex monomials, the following depictions are presented for the first several monomial terms.

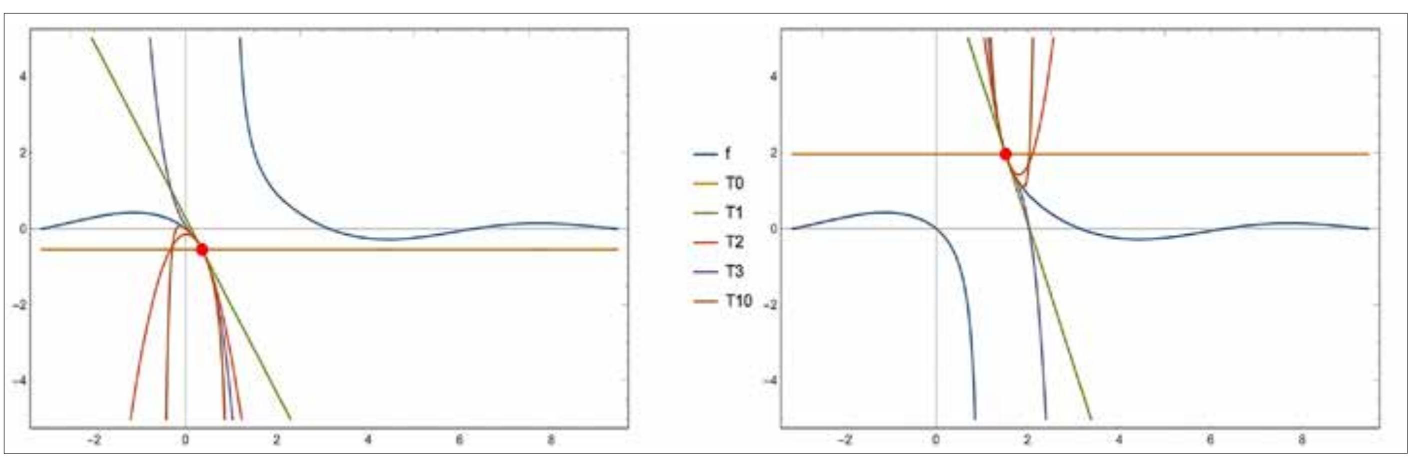

Figure 1 - A depiction of a function $f(x) = \frac{sin(x)}{(x-1)}$ with a singularity at $x = 1$ evaluated at $x = 0.5$ (left) and $x = 1.5$ (right).

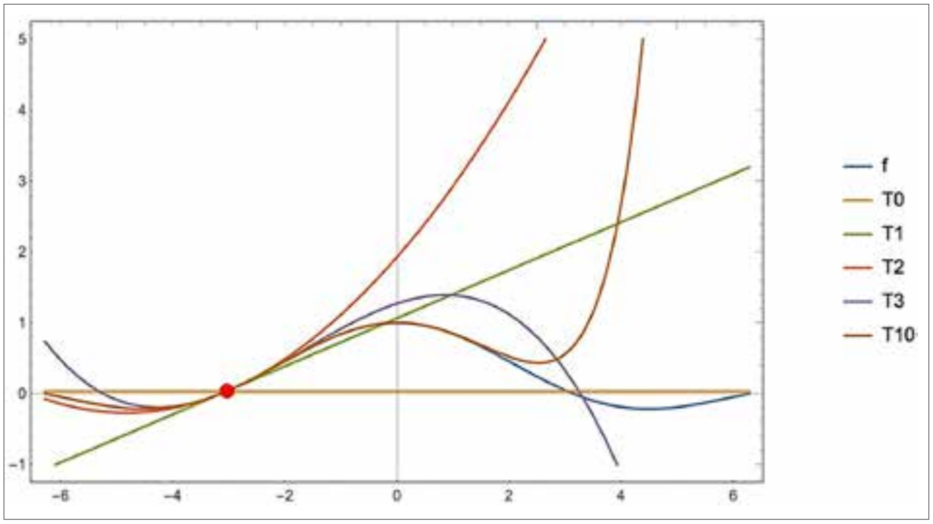

Figure 2 - A depiction of function without a singularity evaluated at point $x = -3$.

It is noteworthy that these individual flow net diagrams can be combined via the Taylor Series formulation as in a partial sum construction and plotted, resulting in a flow net corresponding to the partial sum. Shown in the following is the evolution of the partial sum flow net with increasing numbers of terms in the Series for the classic complex analytic function e^z. It is noted that these partial sum flow net visualizations are combinations of the individual complex monomial flow nets, weighted according to the complex derivative term values evaluated at the selected expansion point.

In the Taylor Series formulation, we determine the entire spectrum of complex variable derivatives and then evaluate at a selected expansion point, Z_0, that is held constant for the evaluation of the entire series. Of course, the entire spectrum of terms involving complex derivatives is evaluated at the chosen expansion point. The complex monomials that are also evaluated with respect to the chosen expansion point, Z_0, depend on the chosen expansion point location.

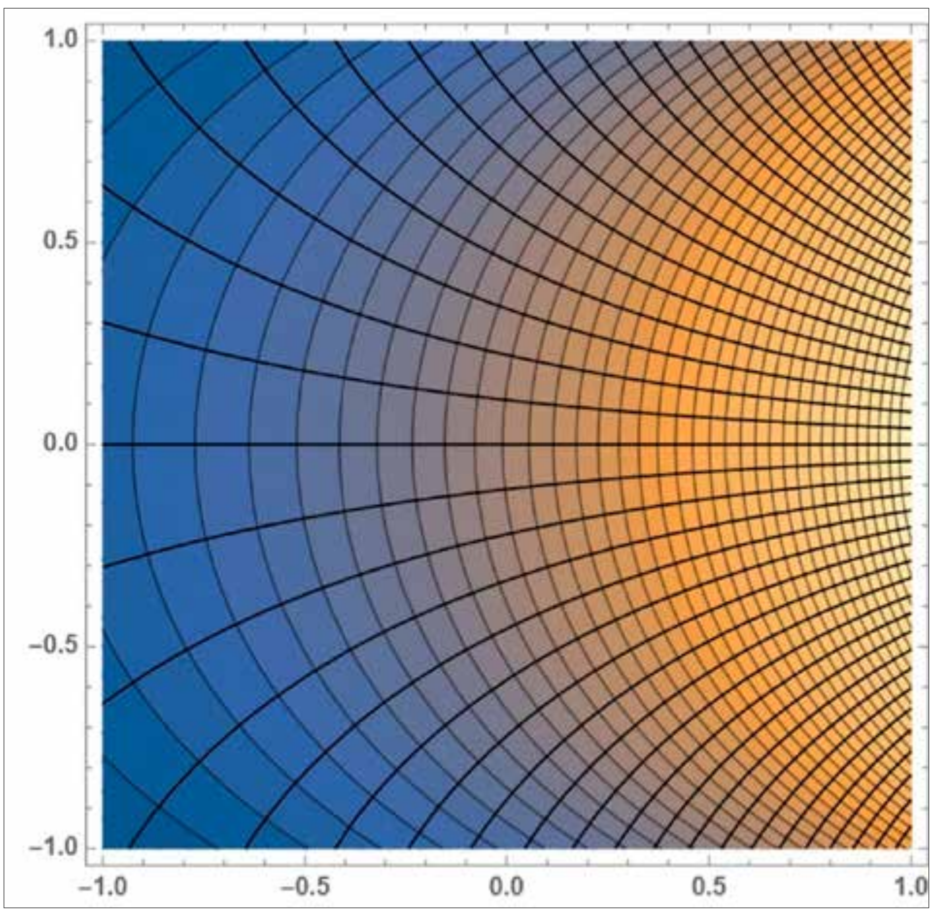

Figure 3 - The exact flow net for the function e^z on the domain [-1,1].

Figure 3 demonstrates the flow net for the exact solution. We present this to show what, in theory, the Taylor Series partial sum approximation flow net should look like as well once the approximation includes a sufficient number of terms. The series of four flow nets in the figure below demonstrates how quickly the addition of terms can model a complex example of the Taylor Series partial sum approximation. With only four terms, the graphic is nearly identical to the exact solution.

When comparing the flow net for four terms (the bottom right portion of Figure 4) to the flow net for ten terms (Figure 5) on page 60, it becomes apparent that there is a diminishing return beyond the fourth term in this instance.

The computational power required to solve a Taylor Series approximation is much less than that needed to find an exact solution. Some complex problems would require exact solutions that take hours or even days for a machine to solve, when a Taylor Series approximation to the fourth term, for example, is much more rapid. The saved computing time translates to both monetary savings and the creation of potential to address other problems.

Suggested Future Work

There are several key topics that need additional research. For example, multiple dimension Taylor Series would be important to apply in order to identify detailed aspects that require further work to resolve. Additionally, inclusion of the time derivative in a Taylor Series expansion may help improve upon the research. Another step towards proper development and application of such models is to apply all coefficients from a complete Taylor Series at a single expansion point. Observing how the total function performs with such information is still under investigation. Other topics are readily available for further research as well.

Conclusions

It is readily noticed that in order to develop the relevant Taylor Series partial sums that the solution to the governing equations must be known. However, using the graphical visualization of the

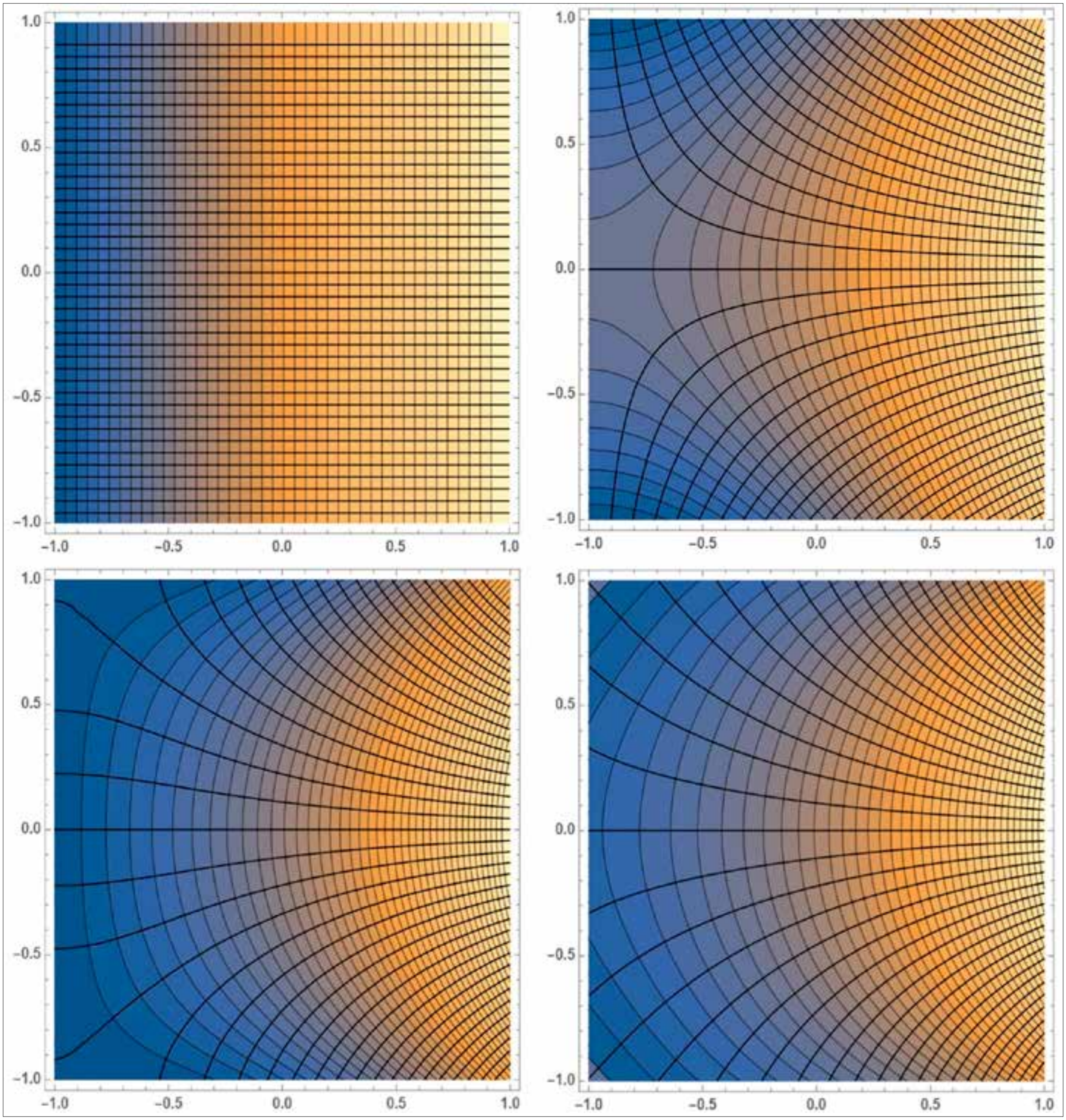

Figure 4 - The Taylor Series approximation of function e^z with one term (top left), two terms (top right), three terms (bottom left), and four terms (bottom right).

partial sum, estimates of these derivative terms at the selected expansion point can be developed by "fitting" the approximation flow net boundary iso-contours to the known problem boundary conditions iso-contour. This is a procedure called the "approximate boundary" fitting to the true problem boundary and involves a graphical visualization of computational error. The measure of "goodness of fit" between the complex approximation (partial sum) and the problem solution is the "goodness of fit" between the partial sum flow net and the problem boundary conditions.

The ability to use methods such as this one will allow use of non-standard modeling methods to determine more accurate approximations in problems dealing with geoscience topics such as groundwater flow estimates.

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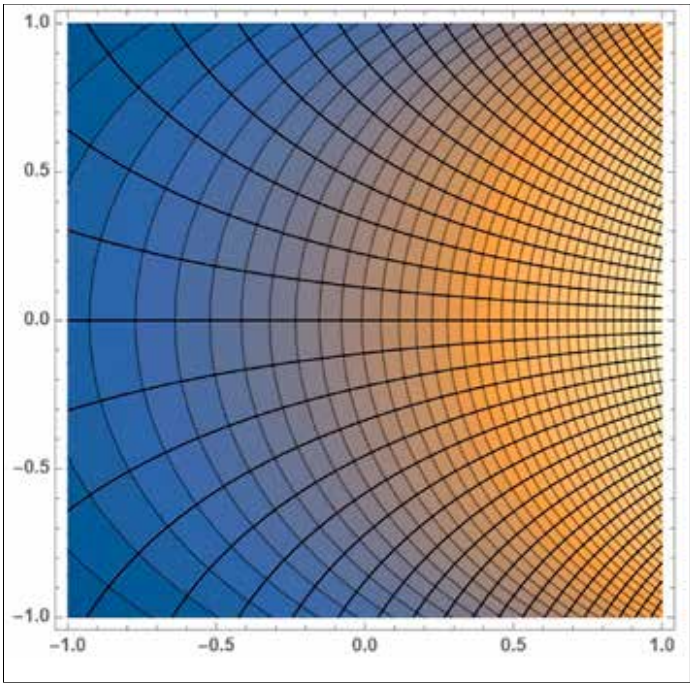

Figure 5 - The ten term Taylor Series partial sum approximation for the function e^z.

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