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THE FUTURE OF ANALYTICAL SOLUTION METHODS FOR GROUNDWATER FLOW AND TRANSPORT SIMULATION

James R. Craig*, **W. Wayne Read**†

*Department of Civil & Environmental Engineering
University of Waterloo, Waterloo, ON, Canada
e-mail: jrcraig@uwaterloo.ca, web page:http://www.civil.uwaterloo.ca/jrcraig/

†Department of Mathematics & Statistics
James Cook University, Townsville, QLD, Australia
e-mail: wayne.read@jcu.edu.au

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Summary. The authors here posit that a renaissance of analytical and hybrid analytical-numerical solutions may be forthcoming. Despite the small number of researchers developing analytical solution approaches, techniques are steadily becoming more and more flexible and robust. Analytical modelling techniques, including convolution, transformations, analytic elements, and series solutions, are being used to augment, complement, or replace discrete models in order to solve specific and relevant problems ranging from carbon sequestration to surface water-groundwater interaction to reactive transport modelling. The authors here first ask and answer the essential question: "what is an analytical solution?". This is followed with a presentation of multiple recent advances in analytical modelling approaches, some necessary ingredients for future success, and some reasons why we might want to see analytical and semi-analytical approaches succeed.

1 INTRODUCTION

Up until the mid-to-late 1970s, discrete numerical solutions to complex groundwater problems were in their infancy. They were deemed correct only if they could match an analytical solution with some desired degree of accuracy. However, the ability of finite element and finite difference approaches to simulate complex problems with irregular geometry, non-linearity, and complex boundary conditions soon outstripped what was then feasible with analytical approaches. Further development of analytical solutions was relegated to a curiosity, and a golden age of discrete numerical methods was ushered in. In the meantime, with increased computational power, improved algebraic manipulation packages, and a bit of progressive creativity, the nature (and perhaps the definition) of analytical solutions has changed rather significantly. This evolution has blurred the boundary between 'analytical' and 'numerical' and led to some novel and powerful tools for understanding groundwater systems. In the last 20 years, analytical methods have become increasingly advanced. Water resource scientists and engineers have paired up with mathematicians, developing both application-specific and general solutions that rely upon methodologies previously inaccessible or intimidating to non-mathematicians, such as Lie symmetry analysis, homotopy methods, and perturbation approaches. Likewise, 'old tricks' have been re-purposed to solve new problems in unique and interesting ways. Below, we discuss the softening boundary between analytical and numerical solution methods, inventory some noteworthy advances from the last quarter century, and discuss the future of analytical methods in water resources.

2 WHAT IS AN ANALYTICAL SOLUTION?

It is typically understood that any exact solution to a differential equation (DE) that can be expressed in terms of polynomial, logarithmic/exponential, and/or trigonometric functions is an analytical solution. Likewise for solutions expressed in terms of special functions (e.g., Bessel, Airy, or Error functions). This library of so-called "closed-form" solutions which can be both derived and evaluated on paper with nothing but Abramowitz and Stegun[1] by one's side comprises the bulk of the literature on analytical solutions to subsurface flow and transport problems. Despite the significant utility of the closed-form Theis or Ogata and Banks equations, most such solutions are of limited scope and applicability due to the restrictions on boundary conditions, dimensionality, or other assumptions.

Over the past thirty years, as personal computers have become commonplace, the definition of 'analytical solution' has shifted. Solutions to DEs can now be automatically generated from symbolic manipulation packages such as Maple, and are typically too sophisticated to be evaluated without a computer. Once the solution can no longer be evaluated by hand, the distinction between numerical and analytical starts to blur. What if the mathematical solution is an unnamed integral, hypergeometric function, or can only be expressed in implicit form? What if numerical integration or root-finding algorithms are required to evaluate the solution? What if, to calculate the coefficients of a series, we have to numerically solve a system of linear algebraic equations? Numerically invert from Laplace space? Are these no longer analytical solutions? The authors are inclined to suggest otherwise.

We here propose the following definition:

- **Analytical solution (n) [an′ə-lĭtĭ-kəl sə-′lü-shən]: any solution to a differential equation that can be evaluated to any desired degree of accuracy at a given point in space and time, without modifying the structure of the solution**.

The precision at which we evaluate derivatives, integrals, and the function itself can be determined and bounded, i.e., we can precisely estimate any error in the solution due to (for example) series truncation or round-off. This definition includes any function that can be approximated to any degree of accuracy using a truncated Taylor series approximation, whether this is done on computer or by hand. Note that under this definition, solutions in Laplace or Fourier space that require numerical inversion, solutions built from infinite sums, solutions that require the solution of systems of algebraic equations or solutions expressed as integrals with known integrands are validly analytical, despite the fact that they are often dubbed 'semi-numerical' or 'semi-analytical'.

Semi-analytical methods are here defined as those approaches which do not meet the definition of analytical methods above, but still utilize the mathematical tricks of analytical solution derivations (e.g., superposition, coordinate/variable/integral transforms, etc.) to help refine or augment the numerical approximation. Semi-analytical methods may be analytical in space and numerical in time, or locally analytical, globally numerical. They may rely on closed-form mathematical transformations to non-physical coordinates. Representative examples in subsurface flow and transport include the Laplace Transform Galerkin method[2] and the semi-numerical solution of Li et al.[3].

Most mathematical methods fall somewhere on the spectrum from purely analytical to purely numerical (see figure 1). It is the authors' contention that the future of numerical methods for flow and transport - the next wave of robust, efficient, and more accurate techniques - lie somewhere in the middle of this spectrum. This includes both descendants of analytical methods improved through use of numerical approximations and descendants of current numerical methods informed by and augmented with analytical approaches.

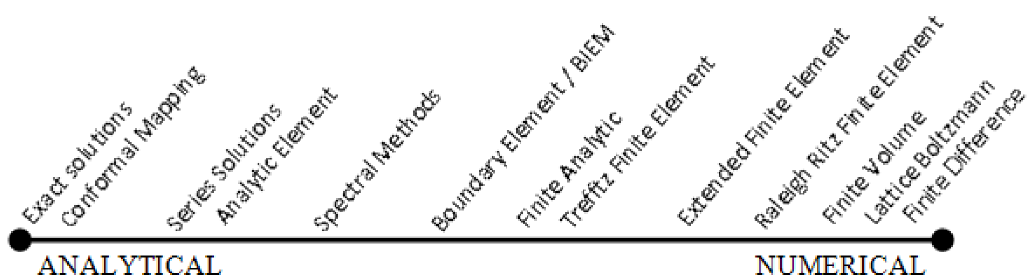

Figure 1: The spectrum of mathematical methods for environmental simulation.

3 NOTEWORTHY ADVANCES

Analytical solutions are often characterized as elegant, but inflexible; charming, but non-robust; at the worst, complicated beyond understanding. While there are certainly many examples to support this characterization (indeed, the authors grow tired of evaluating such solutions in the peer-review process), there are many classes of problems where an analytical or semi-analytical approach provides greater understanding, faster computation, and/or more accurate solutions. The scope and complexity of water resource problems that may be solved using these approaches only increases with time. Where a "purely analytical" approach is infeasible, numerical solution techniques can learn from the tricks and transformations employed to solve simpler problems analytically. Here, a number of general categories of problems are posed, and examples from the literature are referenced. The review focuses on relatively flexible analytical methods with general applicability rather than single-use solutions.

3.1 Problems of Scale

Geographic scale is still a significant computational hurdle in our field. Worthwhile problems of flow and transport often require resolution of regional scale problems that may be impacted by local-scale phenomena. Numerical methods that can resolve both without the use of brute force computation are still the exception rather than the rule, and problems of mixed scale can sometimes be limited by the quality of the mesh generator rather than the inherent speed of the numerical solvers. In response, some researchers have attempted to remove the need for spatial discretization through clever use of analytical tools. A key example is that of the analytic element method (AEM)[4], initially developed during the early 1980s, which relies upon the superposition of infinite-domain analytical solutions to a given governing equation, each with some degrees of freedom. While the solutions themselves always satisfy the governing equation at every point in the domain, a solution technique is needed to identify these unknown coefficients such that the boundary conditions are also met. Since its initial application to steady-state flow in single-layer aquifers, the AEM has been extended to transient [5], 3-D, multi-layer[6], and unsaturated flow[7] problems. This extremely accurate method has far exceeded the capabilities of numerical methods in at least one significant area: the use as a numerical laboratory for dispersion testing[8]. Using AEM, particle advection through more than 100,000 three-dimensional ellipsoidal inclusions in conductivity could be simulated with flow errors on the order of machine precision, enabling the testing of classical theories of dispersive transport and the effective conductivity of heterogeneous media. With the use of Wirtinger calculus, novel new advances are being developed to accurately solve even more challenging problems of multiaquifer and transient flow[9].

The AEM belongs to a more general class of Trefftz methods, in which the governing equation is met exactly and the boundary conditions met with high accuracy (sometimes to machine precision). A cousin of AEM, researchers have used finite-domain series solution methods to study saturated and unsaturated flow in hillsides with complex geometry[10] and to simulate regional-scale topography-driven flow[11, 14], as shown in figure 2.

Another remarkable recent advance is the use of superposition of analytical solutions to determine risk of leakage in multilayer sedimentary aquifers subjected to injection of Carbon for sequestration purposes[13]. The speed in which the multi-scale problem can be solved analytically for multiple realizations is invaluable for risk assessment, and is simply infeasible using standard discrete numerical methods.

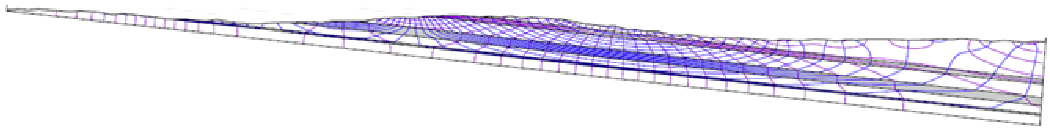

Figure 2: Flow net for topography-driven flow in a mutltilayer aquifer using the series solution method of Craig (2008)

3.2 Problems of Time

Groundwater flow and transport models are expected to predict environmental change over increasingly long time scales. Investigation of climate change or radioactive waste storage can require simulation durations of hundreds of years. It is now routine to use solute transport simulators to estimate the evolution of contaminant plumes at the decadal time scale. As advocated by Olsthoorn[17], one of the most powerful analytical tools we have to address problems of time is that of convolution. For linear or-near linear problems, the use of convolved impulse response functions can significantly reduce computational time and provide improved insight into the nature of the physical problem, at reduced computational cost. This benefit is not limited to analytical models; even complex numerical models may be used to determine the impulse response. Clever approaches, such as the one used by Bakker et al.[16], rely upon convolution and moment matching to transform the transient problem into an equivalent steady state problem, much like is done in the Laplace transform domain, but without the difficulty of inversion.

3.3 Problems of Geometric Complexity

Historically, one of the most salient limitations of analytical solutions has been the restrictions on system geometry. Finite element and finite difference methods can conform to arbitrary material and external boundary geometry. Purely analytical solutions are traditionally limited to rectangular, homogeneous domains. However, both the analytic element method [4] and series solution methods[10, 14] have recently been successfully applied to systems with quite complex shape, without requiring volumetric discretization. Series solution methods actually improve in performance and accuracy with increasing aspect ratio of the modeled domain, unlike most numerical methods. Lastly, they are quite adept at solving the free boundary condition at the water table, a historically challenging problem for analytical and numerical methods alike.

3.4 Problems of Sophistication

A likely source of future innovation may hide in the vast library of mathematical tricks historically used by analyticians to solve single-application problems. These tricks are rarely appropriated by numerical methods researchers. Perhaps the most promising of these is the use of coordinate, variable, and integral transforms, which can be used to reduce the order or non-linearity of a problem statement and therefore improve model convergence, speed, and stability. For example, De Simoni et al.[18] have demonstrated that complex mixing-based problems of geochemical equilibrium in dispersive transport can be solved (sometimes analytically) by re-expressing the problem into one stated in terms of conservative quantities. Ji et al.[19] successfully used variable and integral transformations in order to develop a more robust means for solving the three-dimensional transient Richards equation. Sun and Clement[20] utilized a transform to significantly simplify the simulation of parent-daughter decay chains, which has since been generalized to very complex reaction networks. There are likely many more similar, but untapped, transformation techniques that can be 'borrowed' by numerical method developers in order to more robustly solve the complex and challenging problems of stability and convergence that plagues fully three-dimensional transient non-linear systems of PDEs used to describe multi-species reactive transport, multiphase flow, and unsaturated water flow.

4 CHALLENGES

There are a number of issues that impede both our ability to model general systems with purely analytical methods and our ability to move forward in the development of robust semi-analytical methods. The most salient obstacle, perhaps, is that of non-linearity. Most solutions to non-linear DEs are highly specific and of low dimension. However, applied mathematicians and engineers have long recognized the power of transformation, and we have already begun to see powerful applications of Lie symmetry analysis[22] and Adomian's decomposition method[9] to problems of porous media flow and transport. Newer mathematical techniques such as the inverse scattering transform, homotopy analysis[21] and homotopy perturbation[23] have recently been introduced to the mathematical literature, and may show promise in reducing the non-linearity of flow and transport problems, first in one dimension, then hopefully in higher dimensions.

Non-uniformity of differential equation coefficients is another obstacle to general extension of purely analytical techniques. Current methods are only efficient for some specific forms of non-uniformity (e.g., separable material properties), via clever transformation of variables and/or coordinates. The above methods designed to handle non-linearity can also be used for problems of non-uniformity, but general application is still years away.

5 CONCLUSIONS

The benefits of introducing more analytical tools and sensibilities into our numerical methods are clear: the availability of error estimates, combined with increased efficiencies for many types of multi-scale, unstable, and/or non-linear problems, makes the hybridization of numerical and analytical approaches promising. Likewise, purely analytical approaches, such as analytic element, spectral, and series solution methods are growing more powerful in their own right as the small group of analyticians slowly hammer away (in their own unique manner) at the difficult problems faced by our field. The term 'analytical' should no longer be considered synonymous with 'limited', but should rather be recognized as a worthy goal toward which numerical methods may wish to strive toward. The next generation of analytical and hybrid numerical/analytical methods can be expected to build upon the successes in the previous 10 years, and the authors look forward to see what treasures that might bring.

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