Solving water pollution problems using auto-Bäcklund transformations

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Abstract

In this work an analytical formulation for solving partial differential equations is proposed. The method dispenses the use of Lie groups to produce maps between exact solutions, and generates nonlocal symmetries admitted by differential equations. The method is applied in water pollution problems, furnishing exact solutions for the advection-diffusion equation which describes the propagation of bacteria and chemicals in water bodies with arbitrary contours.

1 - Introduction

Solving water pollution problems are the first step to prevent environmental damages caused by industrial activity and domestic sewers along rivers and lakes. The simulation of water pollution scenarios provides crucial informations for lowering the costs demanded to treat the emissions and to improve the projects related to the implantation of new sewer systems. The most usual methods employed to simulate dispersion scenarios are finite differences (often implicit and time-marching schemes), and finite elements (usually based on Galerkin and least squares formulations). These numerical methods present some inconvenient features when applied to multidimensional problems in complex-shaped domains. The first is related to the time processing required to obtain the numerical solutions, which seldom can be accomplished using coarse meshes. The second is due to the difficulties associated with changes in the source terms. For many practical problems in Environmental Engineering one must simulate repositioning of the sewer loads or treatments for reducing the corresponding concentration, in order to evaluate the effect of the resulting concentration profile along the water body, an then decide whether a given change in the configuration of the sewer system can reduce the pollutant emissions in certain regions of interest. Since this application requires the simulation of several combinations of loading positions and concentrations, and each change in the source terms requires a new numerical simulation, the resulting time processing becomes prohibitive for planning sewer system configurations.

In order to surmount this difficulty, a new analytical formulation based on auto-Bäcklund transformations (Zwillinger, 1992) is proposed. These transformations are nonlocal Lie symmetries admitted by a given differential equation (Bluman and Kummei, 1989), i.e., changes of variables that converts exact solutions of the equation into new exact ones through a discontinuous map, while the local Lie symmetries are continuous transformations. In this work these nonlocal symmetries are obtained by means of a generalized split formulation, which will be described in what follows, instead of employing Lie group analysis (Ibragimov, 1995), which is the procedure often adopted for solving partial differential equations. The main advantages of the proposed formulation relies on the resulting time processing, which is about 0.1% of the one required by solving two-dimensional advection-diffusion equations via finite differences (time marching schemes, for instance), the use of streamfunction and velocity potential as curvilinear coordinates in the solution obtained, which extends the application of the proposed method for arbitrary geometries, and the simplicity of the auxiliary equations to be solved, when compared with the so-called determining equations (Olver, 2000) for the coefficients of the generators which constitute the Lie group. Besides, there are many cases when some of the determining equations are more difficult to solve than the original one. Moreover, the Lie group approach requires the solution of an additional set of auxiliary equations which comes from the application of exponentials whose argument contains a linear combination of the generators, obtained after solving the determining equations. These advantages will become clear after presenting the proposed formulation.

2. The auto-Bäcklund transformation

In this section a new analytical method to construct auto-Bäcklund transformations is described. The method is based on a sequence of non-homogeneousous splits for which the source terms appearing in the corresponding systems of differential equations can be readily obtained from any particular solution of the original equation (even the trivial one). The
The novelty of the proposed method relies in the presence of the source term. The methods based on split generates only homogeneous systems of auxiliary equations (Poblanin, 2004). These methods produces solutions which satisfy a very particular set of boundary conditions. In the proposed formulation, an iterative scheme is obtained, in such a way that each iteration produces a new exact solution satisfying a wider set of boundary conditions. In order to start the iterative scheme, let us consider the equation

\[ Lf = 0 \tag{1} \]

where \( L \) is a linear differential operator, which can be written in the following form:

\[ L = A - B \tag{2} \]

in which the inverse of \( A \) is known. Hence, equation (1) can be expressed as

\[ Af = Bf \tag{3} \]

or, equivalently, as a non-homogeneous system of differential equations:

\[ Af = Q \tag{4} \]

and

\[ Bf = Q \tag{5} \]

where the source term must be determined. It will be showed that when the comutator \([A,B]\) is null the source term can be replaced by any exact solution of equation (1). Indeed, applying operator \( B \) over equation (4), it yields:

\[ BAf = BQ \tag{6} \]

Applying operator \( A \) over equation (6) it results

\[ ABf = AQ \tag{7} \]

Subtracting equation (7) by (6) and taking into account the linearity of both operators, the following result is obtained:

\[ [A,B]f = AQ - BQ \tag{8} \]

Therefore, when \([A,B] = 0 \), the source term \( Q \) obeys the same differential equation satisfied by the unknown function \( f \). The former result allows to carry out and iterative scheme which can be recasted in the following fashion:

\[ Af_{k+1} = f_k \tag{9} \]

and

\[ Bf_{k+1} = f_k \tag{10} \]

The system can be solved in a straightforward way. Starting with any particular solution \( f_0 \) of the original equation, which can be even the trivial one, equation (9) is solved, furnishing:

\[ f_{k+1} = A^{-1}f_k + h \tag{11} \]

where \( h \) denotes a function belonging to the nullspace of \( A \). Substituting the solution obtained into equation (10) it results

\[ Bf_{k+1} = BA^{-1}f_k + Bh \tag{12} \]

Equation (12) is often readily solved for the arbitrary elements contained in \( h \). Eventually, this equation must be splitted, producing another system of non-homogeneous differential equations, whose solution is obtained by applying the same procedure already described.

The new solution obtained is then replaced on the right hand side of equations (9) and (10) and the process is repeated. Notice that at each iteration a new exact solution arises. In other words, the procedure above described does not constitute a iterative scheme which converges to a given exact solution. It is important to bear in mind that the iterations stops when the solution obtained becomes flexible enough to satisfy the initial and boundary conditions imposed in a given subdomain. It means that the number and nature of the arbitrary elements (constants or functions) contained in the solution will define the extension of the subdomain in which this solution remains valid. Roughly speaking, the number of iterations determine whether the solution can be used in a “chunk” or in the whole domain.

In the case when \( A \) and \( B \) do not commute, the proposed method must suffer a slight modification, by defining the \( g \)-commutator, denoted by:

\[ [A,B]_g = AgB - BgA \tag{13} \]

where \( g \) is an unknown function. As in the former case, it is easy to show that when the \( g \)-commutator is null and analogous iterative scheme can be performed:

\[ A_{B_k+1} = f_k \tag{14} \]

and
In fact, multiplying equations (14) and (15) by \( g \), applying operator \( B \) over equation (14) and operator \( A \) over equation (15), and finally subtracting the resulting equations, it yields

\[
[A, B]_g f_{k+1} = Af_k - Bf_k ,
\]

(16)

In order to ensure the “g-commutativity” between \( A \) and \( B \), the function \( g \) must satisfy some auxiliary differential equations which are often simpler than the original equation to be solved. Moreover, for most practical purposes, it becomes possible to map the original equation in such a way that \([A, B] = 0\), and even when the operators do not commute there are infinite solutions for the auxiliary equations which comes from the condition \([A, B]_g = 0\).

3. Application in water pollution problems

The propagation of conservative pollutants in rivers and lakes for complex-shaped domains is given by

\[
\frac{1}{D} \frac{\partial C}{\partial \Phi} = \frac{\partial^2 C}{\partial \Phi^2} + \frac{\partial^2 C}{\partial \Psi^2} ,
\]

(17)

Where \( D \) is the mass diffusivity, \( \Psi \) is the stream function and \( \Phi \) is the potential function. In this equation the hydrodynamical boundary layer effects over the concentration profile are not considered, because the boundary layer thickness are negligible when compared to the geographic scale of the water body. In this case the operators \( A \) and \( B \) are given by

\[
A = \frac{\partial^2}{\partial \Psi^2} ,
\]

(18)

and

\[
B = \frac{1}{D} \frac{\partial}{\partial \Phi} + \frac{\partial^2}{\partial \Phi^2} .
\]

(19)

The corresponding system generated by split is written as

\[
\frac{\partial^2 C}{\partial \Psi^2} = Q
\]

(20)

and

\[
\frac{1}{D} \frac{\partial C}{\partial \Phi} + \frac{\partial^2 C}{\partial \Phi^2} = Q .
\]

(21)

Starting with \( Q = 0 \) and solving equation (20) it results

\[
C(\Phi, \Psi) = f_1(\Phi) \Psi + f_2(\Phi) .
\]

(22)

Replacing the former result in the equation (22), an auxiliary equation arises:

\[
\frac{1}{D} \frac{\partial f_1}{\partial \Phi} + \frac{d^2 f_1}{d \Phi^2} + \frac{d^2 f_2}{d \Phi^2} = 0 .
\]

(23)

The equation above produces two new auxiliary equations:

\[
\frac{1}{D} \frac{\partial f_1}{\partial \Phi} + \frac{d^2 f_1}{d \Phi^2} = 0
\]

(24)

and

\[
\frac{1}{D} \frac{\partial f_2}{\partial \Phi} + \frac{d^2 f_2}{d \Phi^2} = 0
\]

(25)

whose solutions are obtained by direct integration:

\[
f_1(\Phi) = c_1 + c_2 e^{-D\Phi}
\]

(26)

and

\[
f_2(\Phi) = c_3 + c_4 e^{-D\Phi}
\]

(27)

Substituting (26) and (27) in (22) the first exact solution is obtained

\[
C(\Phi, \Psi) = (c_1 + c_2 e^{-D\Phi}) \Psi + c_3 + c_4 e^{-D\Phi} .
\]

(28)

Since \([A, B] = 0\), the process can be restarted with

\[
Q = (c_1 + c_2 e^{-D\Phi}) \Psi + c_3 + c_4 e^{-D\Phi}
\]

(29)

which is replaced on the right hand side of equations (20) and (21). Following the same steps above mentioned, a new exact solution arises:

\[
C(\Phi, \Psi) = \frac{1}{6} (c_1 + c_2 e^{-D\Phi}) \Psi^3 + \frac{1}{2} (c_1 + c_3 e^{-D\Phi}) \Psi^2 + (c_1, \Phi + c_2 (-e^{-D\Phi}, \Phi - e^{-D\Phi}) - c_3 e^{-D\Phi} + c_4 (-e^{-D\Phi}, \Phi - e^{-D\Phi}) - c_5 e^{-D\Phi} + c_6) \Psi + c_5 + c_6 (-e^{-D\Phi}, \Phi - e^{-D\Phi}) - c_7 e^{-D\Phi} + c_8
\]

(30)
Although the process can be easily continued, the former solution is suitable to simulate a wide class of water pollution problems since the shape of the domain depends only upon the expressions for $\Psi$ and $\Phi$. In order to write the solution in the original variables, it becomes necessary to define the streamfunction and the velocity potential. The stream function near an arbitrary contour is given by

$$\Psi(x, y) = U_{\infty} \cdot y + a \arctan \left( b (y - m(x)) \right),$$  \hspace{1cm} (31)

where $a$ and $b$ are numerical parameters which accounts for the mean declivity of the margins, and $m(x)$ is the function describing (locally) the countors. The velocity potential, which is obtained by means of the Cauchy-Riemann conditions (Churchill, 1975),

$$\frac{\partial \Phi}{\partial x} = \frac{\partial \Psi}{\partial y},$$ \hspace{1cm} (32)

and

$$\frac{\partial \Phi}{\partial y} = -\frac{\partial \Psi}{\partial x},$$ \hspace{1cm} (33)

results

$$\Phi(x, y) = U_{\infty} \cdot x - \int \frac{\partial f(x, y)}{\partial x} \, dy + k.$$ \hspace{1cm} (34)

4. Results and conclusions

The proposed method was applied to obtain two-dimensional concentration distributions along the Guaiba lake (Figure 1), by solving equation (17), with boundary conditions of second kind imposed along the margins ($\Psi = \Psi_0$) and a boundary condition of first kind upstream, which specifies the concentration profile at $\Phi = \Phi_0$. In this water body, $a \sim 800$ and $b \sim 0.01$ in equation (31).

The concentration distribution for coliforms, showed in Figure 1, presents reasonably agreement with the experimental data. The mean square deviation between numerical and experimental values is about 20%, the same magnitude of the dispersion between the own measurements.

Figure 1 – Concentration distribution for coliforms (org/100ml)

Figure 2 shows the concentration distribution for phosphorus ($PO_3$ and $PO_4$ forms). In this case, the mean square deviation are roughly about 10%, which is also the same uncertainty verified between the experimental data.

<table>
<thead>
<tr>
<th>Concentration (org/100ml)</th>
<th>Color</th>
</tr>
</thead>
<tbody>
<tr>
<td>less than 200</td>
<td>blue</td>
</tr>
<tr>
<td>200 to 1.000</td>
<td>green</td>
</tr>
<tr>
<td>1.000 to 4.000</td>
<td>yellow</td>
</tr>
<tr>
<td>4.000 to 10.000</td>
<td>orange</td>
</tr>
<tr>
<td>10.000 to 50.000</td>
<td>red</td>
</tr>
<tr>
<td>greater than 50.000</td>
<td>black</td>
</tr>
</tbody>
</table>
Figure 2 – Concentration distribution for phosphorus (mg/L)

In both cases, the time processing required to perform the simulations is about 5 minutes (Sempron 2.8 GHz, 512 Mb RAM, using Visual Basic 6.0).

References