Semi-Lagrangian Numerical solution for Point Source Contaminants Transport in Semi-infinite Homogenous Porous Medium

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1 Introduction

Many activities in modern society produce a large number of dangerous wastes, which pose threats to the environment, and on many occasions, it results in contamination of groundwater. Water may lose quality as a result of pollutants discharge at point sources such as septic tanks, mine spoils, or accidental deposit of contaminants to the ground (Yadav & Jaiswal, 2011). It is known that advection-diffusion partial differential equation equations describe the behavior of pollutants when they invade groundwater from the point source. These equations are difficult to solve for an extended period because they pose restricting conditions for time and spatial stepping to have stability in most numerical algorithms (Süli & Ware, 1991).

Here we would like to study the use of the spectral Semi-Lagrangian method in solving the advection-diffusion equation describing the behavior of the contaminants. Semi-Lagrangian methods are based on combining the spectral method in the spatial variables together with explicit time-stepping along the characteristics (Süli & Ware, 1991). These methods allow for significantly large time steps at almost zero to no costs to the accuracy. The unconditional stability is not only an ideal property to the problem considered here, but in general for most problems in Geosciences as they require tracking the solution for extended periods (Cheney & Rivlin, 1976). The unconditional stability and spectral accuracy of the Semi-Langrangian method is the motivation of the present work. In addition, sources agree that the method can capture the arrival time better than other typically used methods such as the finite difference and finite volume methods. Suppose contaminants have accidentally ended up in groundwater, the need to capture the arrival time of the pollutants to the water bodies that people and livestock may use can never be overemphasized.

The semi-Lagrangian method utilizes interpolation in the spatial variables. In this work, we will use barycentric interpolation at Chebyshev points. Barycentric interpolation at Chebyshev points is known to have excellent stability properties, and exponential convergence (Berrut & Trefethen, 2004; Trefethen, 2019) which motivated our decision to use them in our algorithm.

2 Model description

Figure 1 taken from (Patil & Chore, 2014) shows that after the introduction of the contaminant to the groundwater, it will tend toward the bottom of the aquifer. The concentration gradient drives this motion; pollutants are moving from high concentration to low concentration. The pollutant also disperses in the horizontal direction, whose evidence is the widening of the plume as particles are advected in the plane in the direction of the unsteady flow. Given any point source of the pollutant, the longitudinal and lateral directions in the horizontal plane that extend to infinity where the concentration is zero at any given time (Yadav & Jaiswal, 2011). We can describe the transport of this contaminant using the advection-diffusion equation given as (Yadav & Jaiswal, 2011),

$$\frac{\partial q}{\partial t} + u(t)\frac{\partial q}{\partial x} + v(t)\frac{\partial q}{\partial y} = D_x\frac{\partial^2 q}{\partial t} + D_y\frac{\partial^2 q}{\partial y} - \gamma(t)q. \tag{1}$$

Here u $[LT^{-1}]$ and v $[LT^{-1}]$ are components of flow velocity in the horizontal and lateral directions, and $D_x[L^2T^{-1}]$ and $D_y[L^2T^{-1}]$ and D_y $[L^2T^{-1}]$ are diffusion parameters in the horizontal and lateral directions respectively. The parameter γ $[T^{-1}]$ describes how much contaminants are lost from the plume through factors such as sedimentation. Furthermore, $q(x, y, t)$ is the concentration of the contaminant at any time in the horizontal plane.

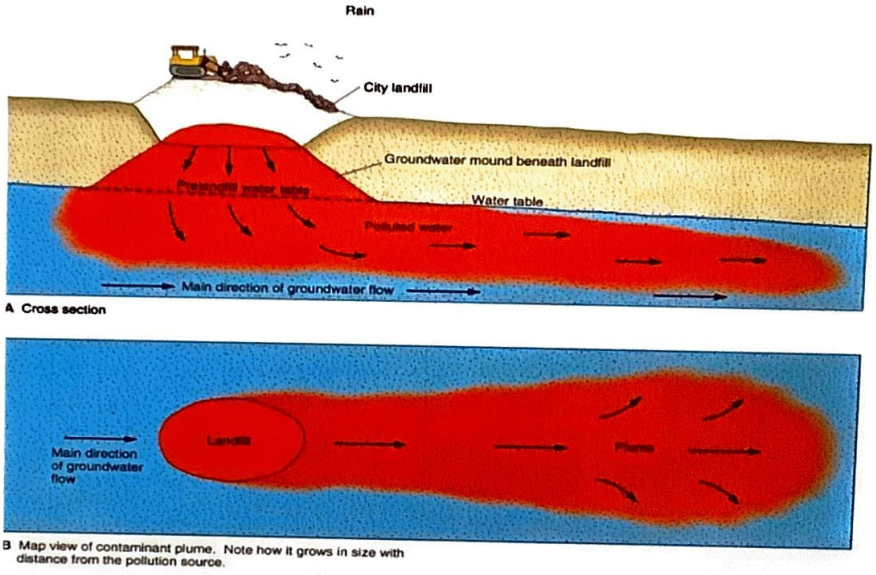

Figure 1: Illustration of contamination of ground water

2.1 Numerical solution

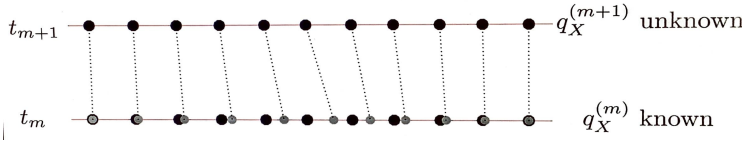

Figure 2: Spatial representation at times t_{m+1} and time t_m

Algorithm 1 Semi-Lagrangian(SL) advection scheme

Input: velocity field $\mathbf{u}(t)$; initial concentration; $X = \{\mathbf{x_j}\}_{j=1}^N$; final time t_f; time-step Δt.
Set $\mathbf{q}_X^0 = \{q(\mathbf{x_j}, 0)\}_{j=1}^N, t = 0$, and $m = 0$.
while $t \leq t_f$ **do**
For $j = 1, \ldots, N$ trace back $\mathbf{x_j}$ in time t to find departure point ξ_j^m.
Set $\mathbf{q}_X^m$to $\Xi^m = \{\xi_j\}_{j=1}^N$ to obtain $\mathbf{q}_\Xi^m$.
set $\mathbf{q}_X^m = \mathbf{q}_\Xi^m, m = m + 1$, and $t = m\Delta$.
end while

To solve (1) we use Semi-Lagrangian (SL) technique. The idea behind the SL method is to use a Lagrangian frame to find the upwind directions for the motion of concentration q (Süli & Ware, 1991;

Shankar & Wright, 2018).To accomplish this we assume that the Lagrangian parcel will arrive at each Eulerian node carrying some concentration of the contaminant q. This concentration q at this grid point is brought from some point of departure so we have to trace back the parcel along the vector field $\mathbf{u} = (u(t), v(t))$ and determine the concentration at the departure point through interpolation. We summarize the the Semi-Lagrangian algorithm of solving (1) using the aid of Algorithm 1 (Shankar & Wright, 2018).

In this study, to interpolate, we use polynomial barycentric interpolation. So to have good stability properties for the interpolants, we use Chebyshev points of the second kind for the fixed set of Eulerian nodes required by the scheme over the entire domain used for interpolating the advected concentrations. Since the Chebyshev nodes of a second kind are given in the domain $[-1, 1]$, in order to cover our domain, we will scale them as follows:

$$x = \frac{L}{2}\left(-\cos\left(j\frac{\pi}{m}\right) + 1\right), \quad j = 0, \ldots, m,$$

Where L is the length of the physical domain, and m is the number of the Eulerian nodes.

3 Data needs

This project aims to develop a numerical algorithm to solve the numerical model (1). In this kind of problem, we use a benchmark problem that has an exact solution or use we use the method of manufactured solution (Zimmermann, Koumoutsakos, & Kinzelbach, 2001). In our case, we will use a version of (1) whose exact solution is computed in (Yadav & Jaiswal, 2011). In their definition, the velocity components u and v, and parameter are taken as exponential with

$$u = u_0 e^{-mt}, \quad v = v_0 e^{-mt}, \quad \text{and } \gamma = \gamma_0 e^{m t},$$

and the dispersion parameters

$$D_x = \alpha u = \alpha u_0 e^{-mt}, \text{ and } D_y = \alpha v = \alpha v_0 e^{-mt},$$

where α is the coefficient that depends on the channel's geometry and average pore size.

Also, we take the initial condition to be

$$q = q_0, \ t > 0, \ x = 0, \text{ and } y = 0, \text{ and}$$
$$\frac{\partial q}{\partial x} = 0, \quad \frac{\partial q}{\partial y} = 0, \quad t \geq 0, \ t \geq 0, \ x \to \infty \text{ and } y \to \infty.$$

It is also given that at time $t = 0$ there are no impurities in the groundwater, that is $q = 0$ (Yadav & Jaiswal, 2011).

The initial velocity components $u_0 = 0.95$ (m/day), $v_0 = 0.095$ (m/day), and coefficient $\alpha = 1.105$ (m) The flow resistance coefficient $m = 0.2$, and the first order of decay term $\gamma_0 = 0.004$ (1/day). We will also run for the steady state case given when $m = 0$.

The exact solution of (1) for these condition is given as (Yadav & Jaiswal, 2011),

$$q(x, y, t) = \frac{1}{2}\left[\exp\left\{\frac{\left(\beta - \sqrt{\beta^2 + \gamma_0}\right)X}{\sqrt{D}}\right\}\operatorname{erfc}\left\{\frac{X - \sqrt{U^2 + 4\gamma_0 DT}}{2\sqrt{DT}}\right\}\right] + \frac{1}{2}\left[\exp\left\{\frac{\left(\beta + \sqrt{\beta^2 + \gamma_0}\right)X}{\sqrt{D}}\right\}\operatorname{erfc}\left\{\frac{X - \sqrt{U^2 + 4\gamma_0 DT}}{2\sqrt{DT}}\right\}\right] \tag{2}$$

where

$$\beta = \sqrt{\frac{U^2}{4D}}, \ D = D_{x_0}\left(1 + \frac{D_{y_0}^2}{D_{x_0}}\right) \ U = u_0 + v_0\sqrt{\frac{D_{y_0}}{D_{x_0}}}, \ X = x + y\sqrt{\frac{D_{y_0}}{D_{x_0}}},$$

$T = \frac{1}{m}\left(1 - e^{-mt}\right), \quad D_{x_0} = \alpha u_0$, and $D_{y_0} = \alpha v_0$. And also erfc is the **complementary error function**, which is defined as

$$\operatorname{erfc}(z) = \frac{2}{\pi}\int_z^\infty e^{-t^2}\mathrm{d}t.$$

4 Calibration or Validation

We will use Heun's method to trace back the particle locations X to find the departure points in our simulations. Furthermore, we use a second-order accurate Backward differentiation formula (BDF2) to integrate in time. The method is theoretically stable, exponentially convergent in space, and second-order accurate in time (Süli & Ware, 1991).

To validate our numerical solution, we utilize the approach used in (Zimmermann et al., 2001) to validate a different numerical scheme to a similar problem. First we will compare the numerical solution q^{nu} to the exact solution (2) (q^{ex}) by plotting the mean squared error

$$\mathsf{MSE} = \frac{\sum_{i=1}^{M} (q_i^{ex} - q_i^{nu})^2}{M-1},$$

where M is the number of particle locations with concentration $q > 10^{-6}\mathrm{g/m}^3$.

The first step is to determine the numerical convergence rates for varied spatial and time step sizes and various magnitude of coefficient for the geometry and pore size of channel α. Here we are trying to determine whether the numerical convergence results agree with the theoretical convergence of the scheme. In addition, we expect the scheme to be stable regardless of the time step size, and we will also run experiments to determine whether this is practically the case for our scheme.

We will also qualitatively assess our numerical solution by comparing the numerical and analytical results' contour plots and breakthrough curves. Qualitative assessments are necessary because estimation errors are not sufficient. There are other things, such as the arrival time of the plume and conservation of mass, which we can not capture by the magnitude of the error.

Lastly, we will determine how our schemes perform as compared to the finite difference method (QUICK scheme) (Slingerland & Kump, 2011). We will compare convergence rates, stability, contour plots, and the breakthrough curves.

5 Numerical experiment design

The experiments aim to determine whether using the Semi-Lagrangian method to solve the transport equation for contaminants in a semi-finite homogenous porous medium is appropriate. A numerical scheme is appropriate for a model if it can give accurate results; we can make the error almost disappear as the step sizes become sufficiently small and if the scheme is stable. Therefore our numerical experiments are designed to test these properties. The experiments will also help us assess the performance of our method as compared to typical techniques for this kind of problem.

5.1 Influence of time step

Here we will run ten experiments using the data provided in section 3 with spatial steps held constant at $\mathrm{d}x = \mathrm{d}y = 5\mathrm{m}$. We will run the experiment for ten years, and we will start with a time step size of fifty days and subtract five each time until five days time step. Theoretically, we expect the MSE to decrease by a quarter each time because the method is theoretically second-order accurate in time; the experiment will determine if that is practically the case. This experiment will also determine if the method is unconditionally stable as we start with very larger time step sizes.

5.2 Influence of spatial step size

Here we fix the time step at $\mathrm{d}t = 1\mathrm{day}$, and we vary the spatial steps equally from 5m to 50m and measure the MSE for each experiment. Here we plot the MSE to determine whether the convergence is indeed algebraic. If it is not algebraic, we investigate the scheme further with different tools to determine where the errors are coming from to adapt our scheme to our problem. Possible sources of errors include interpolating polynomial used and how the differential operator is being applied to the interpolated data.

5.3 Visual investigation of accuracy

Here we try to investigate aspects of accuracy that can not be seen from numerical error. This experiment runs our scheme for different remeshing frequencies and produces contour and breakthrough plots in up to 10 years of simulations. We compare these to similar plots from the exact solution. We observe how much the plots seem to agree with each other visually and determine if the scheme can capture the time of the plume's arrival correctly. The appearance of contour plots at a specific time can tell us more about the conservation of mass and arrival times. The contour plots may look different, yet the error may somehow be small, so this is imperative. So, judging the model based on the error only would be misleading.

5.4 Comparison

Here we run our Semi-Lagrangian scheme and the QUICK method using different remeshing configurations and compare their performances to each other. The areas to compare will include convergence, stability, time of arrival, conservation of mass. The QUICK scheme is a classic in solving transport equations. It is a standard in science to compare new techniques to standard techniques to determine whether they improve existing ones. The new techniques may not improve the old method in all areas but may give better results in some areas, so this comparison would help us decide where the new technique fits in the literature. For instance, if underground water is contaminated with dangerous chemicals, we want to predict the arrival time correctly. In that case, we will go with a scheme that predicts arrival time well.

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