INTERFACES IN POROUS MEDIUM CAPTURED BY LEVEL SET METHODS

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Abstract. *This paper presents the determination of the interface evolution of a tracer (passive scalar) in a porous medium by means of a semi-Lagrangian level set method. Such approach allows for a precise representation of the interface, can handle complex interface evolutions and admits large advancing time steps.*

Keywords. *porous medium, level set method, semi-Lagrangian method, domain decomposition, tracer flow.*

1. Introduction

Models of several scientific and technologic problems present interfaces or boundaries between, for example, different materials, several fluids, or fluids in different states. Some of these boundaries move due to the overall dynamics of the problem in consideration (Ramesh and Torrance, 1993; Strain, 1989; Gonçalves, 1999; Neto, Leme, Souto and Vargas, 1998). Applications range from flame propagation to boiling in porous medium, to mould filling and to ocean waves.

In two dimensions these interfaces are usually represented by one or more closed curves or curves extending to infinity.

Also, there are problems where the curves do not have a motion physically motivated. In computer vision, one is interested in shape detection and recognition. In such problems (Kass, Witkin and Terzopoulos, 1988; Caselles, Kimmel and Sapiro, 1995), motion of an initial curve is driven by properties of the image in order to extract a shape in the image.

Level set methods have been introduced by J. A. Sethian and S. J. Osher (Osher and Sethian, 1988; Sethian, 1996) to describe the evolution of curves. A great advantage of these methods over competing ones is that it treats easily the splitting of a curve in two or more curves and the merge of two or more curves into just one curve. Changes of the topological character of interfaces or boundaries are treated in an unified fashion with a new field variable defined all over the physical domain and which evolves respecting the dynamics of the interface. These methods have been generalised to three dimensions and are easily implemented.

In this work, we apply a level set method, time-integrated by means of a semi-Lagrangian approach, to the study of the motion of a passive scalar in a heterogeneous porous medium. Due to the complex nature of the porous medium, the passive scalar evolves to form a region with a non-trivial geometry which can be handled computationally by a level set method.

In section 2 we present the equation for the flow of a fluid and of a tracer in a porous medium. The basic idea of level set methods are presented in section 3. The solution of the flow problem using a domain decomposition method is presented in section 4. Section 5 shows a semi-Lagrangian implementation of the level set method. Finally in section 6 we present some numerical results and conclusions.

2. Flow of a Tracer in a Porous Medium

We consider the evolution of a tracer in a porous medium. Since the tracer is non-reacting and non-diffusing (passive scalar), its evolution can be followed by its interface with the fluid, see Fig. 1.

The interface evolves by means of the velocity field of the incompressible fluid which satisfies Darcy's law,

$$\begin{aligned} \nabla \cdot \mathbf{u} = f = \delta_{inlet} - \delta_{outlet} \qquad & \text{in } \Omega; \\ \mathbf{u} = -K \nabla p \qquad & \text{in } \Omega; \\ \mathbf{u} \cdot \mathbf{n} = 0 \qquad & \text{on } \partial\Omega. \end{aligned} \tag{1}$$

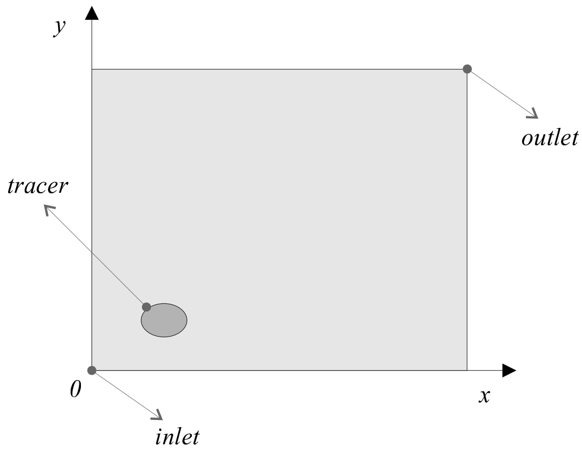

Figure 1: Porous medium filled with a fluid and a tracer.

Here Ω represents the porous region, p is the pressure, $\mathbf{u}$ is the velocity field, K is the permeability, and $f = \delta_{inlet} - \delta_{outlet}$ represents a Dirac's delta source in the inlet position and a Dirac's delta sink in the outlet position.

3. Level Set Method

Level set methods have been introduced by Osher and Sethian (Osher and Sethian, 1988; Sethian, 1996). Their aim is to evolve accurately curves, surfaces, or interfaces subject to a specific dynamics, allowing the treatment of changes in their topological structure, the splitting of an interface in two or more interfaces and the merge of two or more interfaces into just one, easily.

These methods are based on a suitable representation of the interfaces by means of a scalar field, ϕ, the level set function, and in setting up an evolution equation for ϕ which preserves the representation.

We consider the method for interfaces in 2-D represented by curves. Denote by Γ_t the interface (a simple curve or a set of curves) at time t. At each fixed time t, the interface is represented by the null level set of $\phi(\cdot, t)$,

$$\Gamma_t = \left\{ \mathbf{x} \in \Re^2 \mid \phi(\mathbf{x}, t) = 0 \right\} . \tag{2}$$

The evolution equation for ϕ must be compatible with Eq. (2). Let $\mathbf{x} = \mathbf{x}(t)$ denote a point in the interface, $\mathbf{x}(t) \in \Gamma_t$. Assume that the velocity field of the evolving interface is $\mathbf{u}$. Then, by representing by a dot a time derivative, we have

$$\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x}, t) \, . \tag{3}$$

From Eq. (2) we must have

$$\phi(\mathbf{x}(t), t) = 0 \tag{4}$$

and differentiating this equation with respect to time, one gets,

$$\phi_t + \dot{\mathbf{x}} \cdot \nabla\phi = 0 \, . \tag{5}$$

Substituting Eq. (3) into Eq. (5), we finally determine the evolution equation for ϕ,

$$\phi_t + \mathbf{u} \cdot \nabla\phi = 0 \, . \tag{6}$$

To complete the description of the level set method at an analytical level, we need to specify initial conditions for ϕ, compatible with Eq. (2). A simple way to do this is to let $\phi_0(\mathbf{x}) = \phi(\mathbf{x}, 0)$ be a signed distance of $\mathbf{x}$ to the interface; if $\mathbf{x}$ is inside the region delimited by the interface, $\phi(\mathbf{x}, 0)$ is negative, and if $\mathbf{x}$ is outside $\phi(\mathbf{x}, 0)$ is positive (see Fig. 2). For instance, if Γ_0 is a circle, $\Gamma_0 = \left\{ (x, y) \mid (x - x_0)^2 + (y - y_0)^2 = r^2 \right\}$, then we can define $\phi(\mathbf{x}, 0) = \sqrt{(x - x_0)^2 + (y - y_0)^2} - r$. However, for later times, $\phi(\mathbf{x}, t)$ is not necessarily equal to the distance to Γ_t; we emphasize that what remains valid by the evolution defined by Eq. (6) is Eq. (2). Therefore, by finding the zeros of $\phi(\cdot, t)$ for a fixed time t, we determine the interface Γ_t.

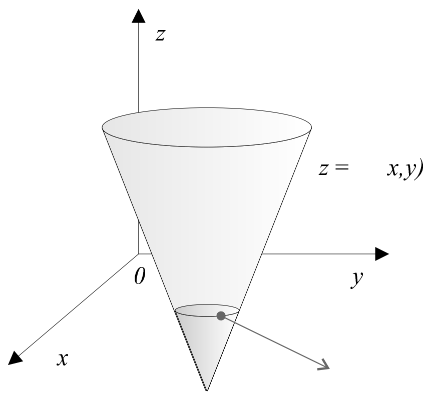

Figure 2: The initial level set function, $\phi_0(x, y)$, is chosen here as a signed distance to the interface Γ_0.

4. Solution of the Flow Problem

The velocity field in the porous region, which is taken as a square, is computed by solving Eq. (1) rewritten here as

$$\nabla \cdot (-K\nabla p) = f = \delta_{inlet} - \delta_{outlet} \qquad \text{in } \Omega \tag{7}$$

for the pressure, by a domain decomposition presented by Douglas et al. (Jr., Leme, Roberts and Wang, 1993). The spatial domain is divided into square cells and, in each cell, nine quantities, representing physical variables, are stored: the values of the pressure at the center of the cell, p, the values of the pressure at the middle point of the edges of the cell, l_R, l_U, l_L and l_D, and the values of the normal components of the velocity field at each edge of the cell q_R, q_U, q_L and q_D (for example, $q_L = \mathbf{u} \cdot (-1, 0)$); see Fig. 3.

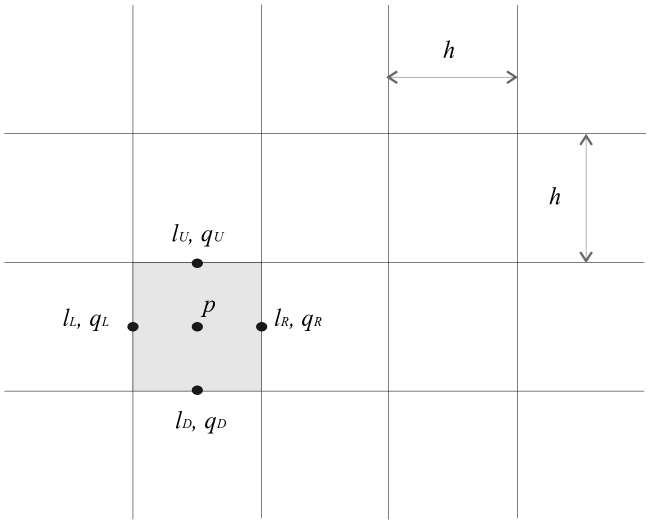

Figure 3: The porous media and its decomposition into square cells.

Integration of the mass conservation equation over a cell, first equation in Eq. (1), leads to its discrete form,

$$q_R + q_U + q_L + q_D = fh \tag{8}$$

and the discrete version of the momentum equation (second equation in Eq. (1)) can be written to each edge as

$$q_\alpha = -\frac{2K}{h}\left(l_\alpha - p\right), \qquad \alpha = R, U, L, D\,. \tag{9}$$

The linear system defined by Eq. (8) and Eq. (9) has 5 equations and 9 unknowns for each cell. To close up the system, coupling equations, Robins interface conditions, are used,

$$l_\alpha = \beta_\alpha\left(q_\alpha + \bar{q}_{\bar{\alpha}}\right) + \bar{l}_{\bar{\alpha}}\,, \qquad \alpha = R, U, L, D\,, \tag{10}$$

where $\bar{\alpha}$ refers to the labelling of the edge by the adjacent cell (for example, $\bar{\alpha} = L$ when $\alpha = R$) and $\bar{q}$, $\bar{l}$ to the values of the physical variables on that adjacent cell. Also, $\beta_\alpha = \beta_{\bar{\alpha}}$ is a constant on the edge chosen empirically to accelerate convergence; it is taken positive to avoid numerical instabilities due to the existence of Steklov eigenvalues in the boundary operator, Eq. (10) (Gustafson, 1987).

Equation (7) together with the boundary condition (third equation in Eq. (1)) does not have a unique solution since an arbitrary constant can be added to p. A unique solution can be specified if it is assumed that the global mean of the pressure is null,

$$\int_\Omega p(x,y)\; dxdy = 0\,. \tag{11}$$

This requirement is accomplished in an update step. Let $\tilde{p}$ be the computed pressure on the cells, $\tilde{l}$ be the pressure field on edges and

$$m = \int_\Omega \tilde{p}\; dxdy \quad \text{and} \quad V = \int_\Omega \; dxdy = \mathrm{Vol}(\Omega)\,. \tag{12}$$

Let p be the global null average pressure field, and l its value on the edges of cells. Then, on each cell, we let

$$p = \tilde{p} - \frac{m}{V} \quad \text{and} \quad l_\alpha = \tilde{l}_\alpha - \frac{m}{V}\,. \tag{13}$$

It is easy to check that p defined by Eqs. (12 – 13) satisfy Eq. (11).

Substituting (10) in (9) and rearranging we get

$$q_\alpha = c_\alpha p - c_\alpha \left(\beta_\alpha \bar{q}_{\bar{\alpha}} + \bar{l}_{\bar{\alpha}}\right)\,, \tag{14}$$

where $c_\alpha = \frac{\eta}{1+\eta\beta_\alpha}$ and $\eta = \frac{2K}{h}$. Adding Eq. (14) in α and using Eq. (8) we get

$$p = \frac{fh + \sum_\alpha \left[c_\alpha \left(\beta_\alpha \bar{q}_{\bar{\alpha}} + \bar{l}_{\bar{\alpha}}\right)\right]}{\sum_\alpha c_\alpha} \tag{15}$$

The iterative algorithm to solve Eq. (8 – 11) is based on Eq. (10), (14), (15) and (13) and can now be described. Start from an initial guess, $\overset{0}{p}$, $\overset{0}{q}_\alpha$, $\overset{0}{l}_\alpha$, in each cell. From Eq. (15), let the right hand side, which depends on information from neighbour cells, be evaluated using values from the previous iteration,

$$\overset{n+1}{p} = \frac{fh + \sum_\alpha \left[c_\alpha \left(\beta_\alpha \overset{n}{\bar{q}}_{\bar{\alpha}} + \overset{n}{\bar{l}}_{\bar{\alpha}}\right)\right]}{\sum_\alpha c_\alpha} \quad \text{with} \quad n = 0,1,2,\ldots$$

Use Eq. (14) to update q_α and Eq. (10) to update l_α,

$$\overset{n+1}{q}_\alpha = c_\alpha \overset{n+1}{p} - c_\alpha \left(\beta_\alpha \overset{n}{\bar{q}}_{\bar{\alpha}} + \overset{n}{\bar{l}}_{\bar{\alpha}}\right) \quad \text{with} \quad n = 0,1,2,\ldots$$

$$\overset{n+1}{l}_\alpha = \beta_\alpha \left(\overset{n+1}{q}_\alpha + \overset{n}{\bar{q}}_{\bar{\alpha}}\right) + \overset{n}{\bar{l}}_{\bar{\alpha}} \quad \text{with} \quad n = 0,1,2,\ldots$$

In each iteration step n, p and l_α should be corrected by Eq. (13). This iteration procedure is carried out up to convergence. The values of the velocity field at the corners of the cells are computed by a suitable average of q_α.

5. Semi-Lagrangian Scheme for the Evolution of the Level Set Function

In this section we describe the scheme that we employ to numerically integrate the evolution equation for the level set function, Eq. (6). This assumes that the velocity field $\mathbf{u}$ is known and that it has been solved by the method outlined in the previous section.

The scheme to solve Eq. (6) uses a standard finite difference discretization for the spatial representation of the level set function and a characteristics based method — a Semi-Lagrangian approach — for time discretization (Russell, 1980; Russell, 1985).

The characteristics (Chorin and Marsden, 1980) of the level set evolution equation

$$\frac{\partial\phi}{\partial t} + u(x,y)\frac{\partial\phi}{\partial x} + v(x,y)\frac{\partial\phi}{\partial y} = 0\,, \tag{16}$$

$0 \le x, y \le L$, $t \ge 0$, are the solution curves of the system of ordinary differential equations

$$\left.\begin{aligned} \tfrac{\partial S_1}{\partial t} &= u\left(S_1(t), S_2(t)\right) \\ \tfrac{\partial S_2}{\partial t} &= v\left(S_1(t), S_2(t)\right) \end{aligned}\right\} t \ge t^*\,, \tag{17}$$

$$(S_1(t^*), S_2(t^*)) = (x^*, y^*) \ .$$

The solution $(S_1(t), S_2(t))$ is the trajectory of (x^*, y^*) and $\phi\left(S_1(t), S_2(t), t\right)$ is constant along time

$$\phi\left(S_1(t), S_2(t), t\right) = \phi\left(x^*, y^*, t^*\right) \ , \tag{18}$$

for $t \geq t^*$. This can be seen by checking that it is null the time derivative of the function on the left hand side of Eq. (18), as a consequence of Eq. (16) and Eq. (17).

Equation (18) is the basis of a method to advance ϕ in time. Consider a time semi-discretization, where the time variable is discretized, $t = k\Delta t$, $k = 0, 1, 2, \ldots$. Assume ϕ is known at time level k, ϕ^k, and that we want to determine ϕ^{k+1}. For any given point $(x, y) \in [0, L] \times [0, L]$, we solve Eq. (17) backward in time to determine (x^*, y^*, t^*) given the final point $(S_1((k+1)\Delta t), S_2((k+1)\Delta t)) = (x, y)$ and letting $t^* = k\Delta t$. From Eq. (18) we get that:

$$\phi^{k+1}(x, y) = \phi(x, y, (k+1)\Delta t) = \phi(x^*, y^*, k\Delta t) = \phi^k(x^*, y^*) \tag{19}$$

This is a semi-Lagrangian scheme for Eq. (16). A numerical procedure is used to determine (x^*, y^*), by solving Eq. (17).

We introduce a finite difference spatial grid, $(x_i, y_j) = (i\Delta x, j\Delta y)$, $i, j = 0, 1, \ldots, N$, with $\Delta x = \Delta y = \frac{L}{N}$.

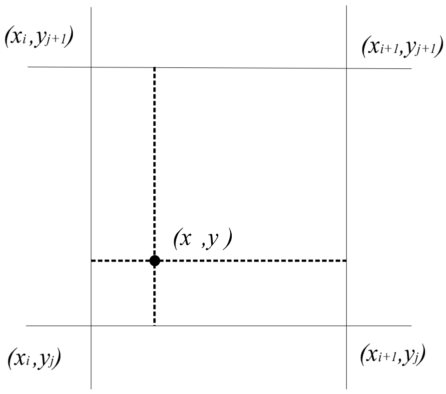

Figure 4: Interpolation of the vector field (u, v). Average linearly the values on (x_i, y_j) and on (x_{i+1}, y_j), and do the same with the values on (x_i, y_{j+1}) and (x_{i+1}, y_{j+1}). Finally average linearly on y those values (see Eq. (23)).

In order to get second order accuracy in the determination of the characteristics which impacts the accuracy of ϕ, we use an implicit method to solve Eq. (17),

$$\begin{aligned} \frac{S_1^{k+1} - S_1^k}{\Delta t} &= u\left(\frac{S_1^{k+1} + S_1^k}{2}, \frac{S_2^{k+1} + S_2^k}{2}\right) \ , \\ \frac{S_2^{k+1} - S_2^k}{\Delta t} &= v\left(\frac{S_1^{k+1} + S_1^k}{2}, \frac{S_2^{k+1} + S_2^k}{2}\right) \ , \end{aligned} \tag{20}$$

with $(S_1^{k+1}, S_2^{k+1}) = (x_i, y_j)$, a grid point. Therefore, substituting in Eq. (20), the value of (S_1^{k+1}, S_2^{k+1}) and of $(S_1^k, S_2^k) = (x^*, y^*)$ which is the unknown, and rearranging we get

$$\begin{aligned} x^* &= x_i - \Delta t\, u\left(\frac{x_i + x^*}{2}, \frac{y_j + y^*}{2}\right) \\ y^* &= y_j - \Delta t\, u\left(\frac{x_i + x^*}{2}, \frac{y_j + y^*}{2}\right) \end{aligned} \tag{21}$$

Given (x_i, y_j) and k, we solve Eq. (21) for (x^*, y^*) by iteration,

$$\begin{aligned} x^*_{r+1} &= x_i - \Delta t\, u\left(\frac{x_i + x^*_r}{2}, \frac{y_j + y^*_r}{2}\right) \\ y^*_{r+1} &= y_j - \Delta t\, u\left(\frac{x_i + x^*_r}{2}, \frac{y_j + y^*_r}{2}\right) \end{aligned} \tag{22}$$

where r is an iteration counter, $r = 0, 1, 2, \ldots$, and we run the iteration up to convergence.

The values of u and v are only known at grid points, $(i\Delta x, j\Delta y)$, $i, j = 0, 1, \ldots, N$, which correspond to cell corners, see section 4. We compute (u, v) in other points by a quasi-linear approximation. Say that we need to approximate (u, v) at (x^ξ, y^ξ) which is located inside the square with vertices (x_i, y_j), (x_{i+1}, y_j), (x_i, y_{j+1}), (x_{i+1}, y_{j+1}). Then

$$\begin{aligned} u(x^\xi, y^\xi) \quad \approx \quad & \left(1 - \frac{y^\xi - y_i}{\Delta y}\right) \left[\left(1 - \frac{x^\xi - x_i}{\Delta x}\right) u_{i,j} + \frac{x^\xi - x_i}{\Delta x} u_{i+1,j} \right] \\ & + \frac{y^\xi - y_i}{\Delta y} \left[\left(1 - \frac{x^\xi - x_i}{\Delta x}\right) u_{i,j+1} + \frac{x^\xi - x_i}{\Delta x} u_{i+1,j+1} \right], \end{aligned} \tag{23}$$

and analogously for $v(x^\xi, y^\xi)$, just exchange u by v in Eq. (23); see Fig. 4.

For improved accuracy in the evolution of ϕ, the value used in the right hand side of Eq. (19) is computed by a quasi-cubic approximation which is determined in the following way, see Fig. 5. We do a linear interpolation

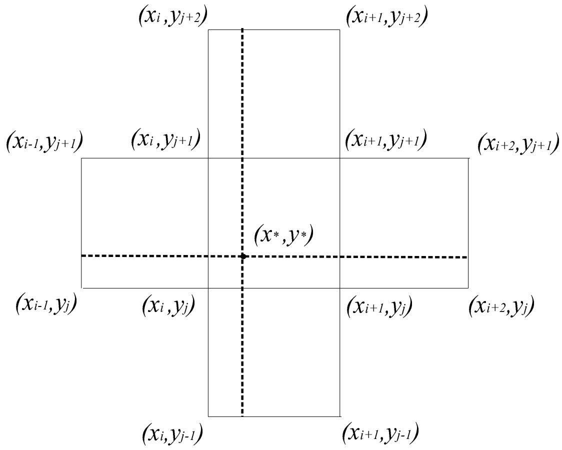

Figure 5: Interpolation of the level set function.

of ϕ in x when $y = y_{j-1}$, a cubic interpolation of ϕ in x when $y = y_j$, a cubic interpolation of ϕ in x when $y = y_{j+1}$ and a linear interpolation in x when $y = y_{j+2}$. Finally, with these four interpolations, we do a cubic interpolation in y.

6. Numerical Results

We consider two types of porous medium, one homogeneous (the permeability K is a constant) and one heterogeneous (with the permeability assuming two values $K_1 = 10^{-14}$ in the middle square, and $K_2 = 10^{-11}$ in the remaining region).

The tracer can either enter continuously into the region by the inlet position or else can be given in the interior of the region as a small blob represented in Fig. 1.

Two numerical methods were used in order to numerically integrate the level set equations, a standard upwind scheme and the semi-Lagrangian method presented in the previous section.

Since the semi-Lagrangian method is CFL-free for stability, it allows larger time steps and it is faster than the upwind method.

The precision on the determination of the tracer-fluid interface is comparable in both methods and in both porous media models, when the tracer enters continuously, see Fig. 7. However, when we consider a tracer blob, the semi-Lagrangian continues to perform well while the upwind method steadily looses the volume of the blob, as one can see in Fig. 6.

In this way we verify that a semi-Lagrangian implementation of the level set method to follow an interface can improve the solution process. This is promising and other problems can benefit from this approach.

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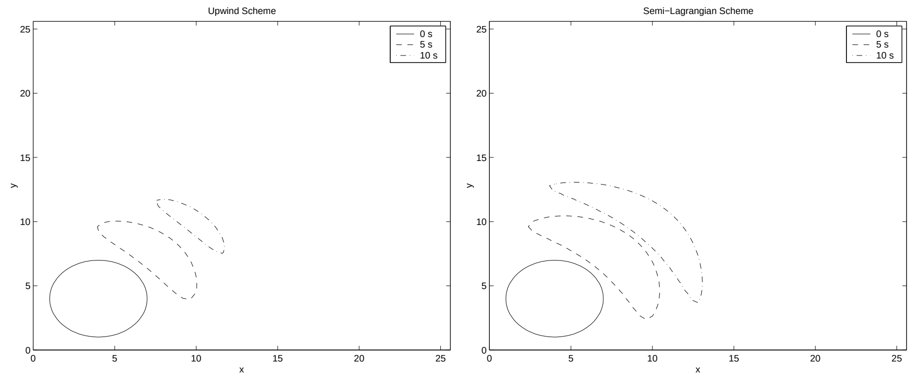

Figure 6: Evolution of a blob in a homogeneous porous medium using an upwind scheme (left hand side) and a semi-Lagrangian method (right hand side). The shape of the blob is plotted at times: $0s$, $5s$ and $10s$.

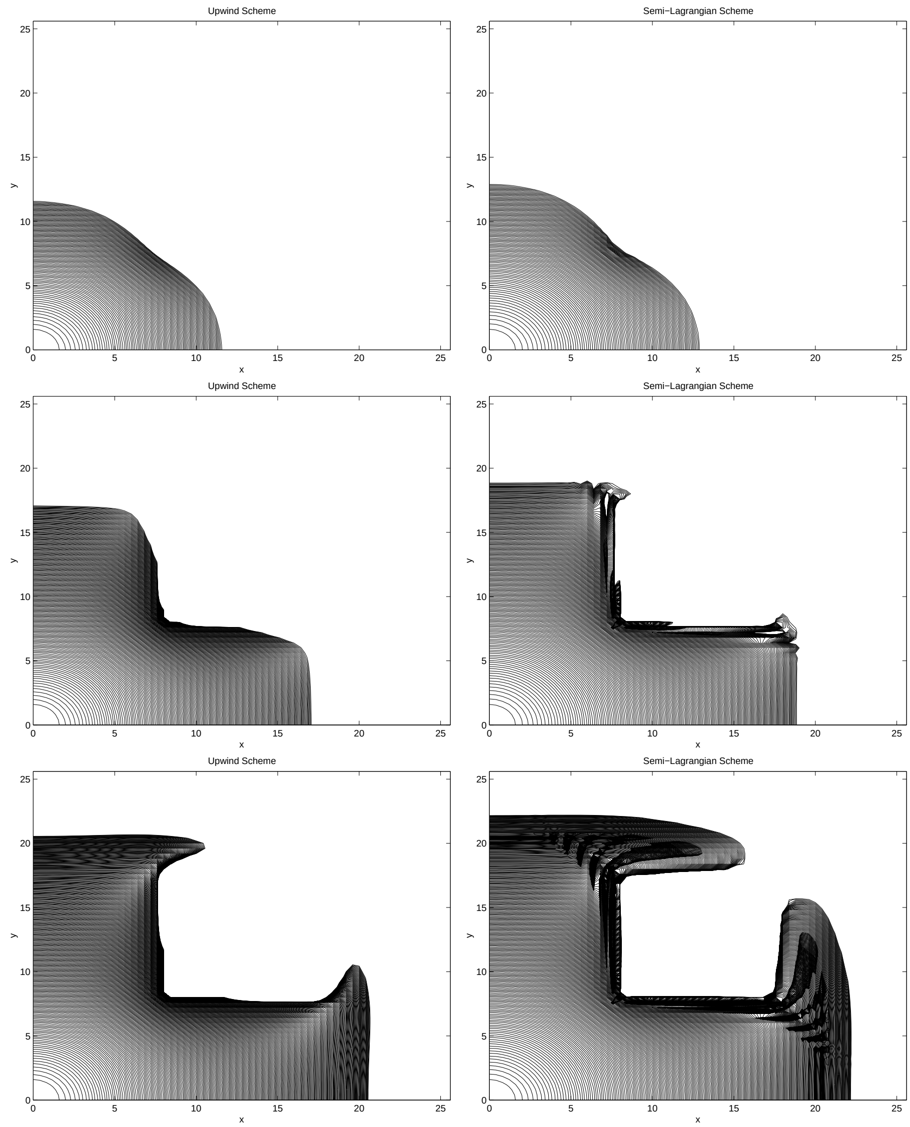

Figure 7: Evolution of a tracer starting close to the inlet position in a heterogeneous porous medium at times: $10s$, $20s$ and $30s$. The graphics on the left hand side represent solutions obtained by an upwind scheme while the ones in the right hand side are computed by a semi-Lagrangian method.

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