MODELLING HETEROGENEOUS BI-DIMENSIONAL SOLUTE TRANSPORT PROBLEMS WITH THE EULERIAN LAGRANGIAN LOCALIZED ADJOINT METHOD

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Key words: ELLAM, oscillations, diffusion

Summary: The Eulerian-Lagrangian Localized Adjoint Method (ELLAM), introduced by Celia *et al.*[1], is an interesting alternative to standard methods to solve advection dominated transport equations. It preserves the performance of characteristic methods and treats general boundary conditions naturally in their formulations.
A new ELLAM formulation was developed by Younes *et al.*[2] for unstructured triangular meshes. This formulation avoids unphysical oscillations and numerical diffusion when several time steps are used. The method requires a very limited number of integration points (usually 1 per element) and is therefore highly efficient. In this work, we show applicability and performances of this method for highly heterogeneous domains containing injection and pumping wells.

1 INTRODUCTION

The incidence of contamination and pollution of groundwater resources demands accurate description and understanding of contaminant transport in porous media. The mathematical model describing transport in porous media is usually an advective-diffusive-equation (ADE) which has the following formulation:

$$\frac{\partial C}{\partial t} + \nabla.(\boldsymbol{V}C) - \nabla.(\boldsymbol{D}.\nabla C) = 0 \qquad (1)$$

with $\boldsymbol{x} \in \Omega$ and $t \in [0, T]$.

Where $C(\boldsymbol{x}, t)$ [M.L^{-3}] is the unknown concentration at location $\boldsymbol{x}$ and time t and $\boldsymbol{D}$ [L^2.T^{-1}] the dispersion tensor defined by

$$D_{ij} = (\alpha_T |\boldsymbol{V}| + D_m)\delta_{ij} + (\alpha_L - \alpha_T)\frac{v_i v_j}{|\boldsymbol{V}|}, \quad i, j = 1, 2 \qquad (2)$$

$\boldsymbol{V}$ [L.T^{-1}] is a given fluid velocity of components v_i and v_j; α_L and α_T [L] are respectively the longitudinal and transverse dispertivities; δ_{ij} is the Kronecker delta function; D_m [L^2.T^{-1}] is the molecular diffusion coefficient and T is the end of the time period starting at time zero.

Equation (1) is subject to the following initial and boundary conditions:

$$C(\boldsymbol{x},0) = C_0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega \tag{3}$$
$$C(\boldsymbol{x},t) = g_1(\boldsymbol{x},t), \quad (\boldsymbol{x} \in \partial\Omega^1, t > 0)$$
$$(-\boldsymbol{D}.\nabla C)\boldsymbol{\eta}_{\partial\Omega} = g_2(\boldsymbol{x},t), \quad (\boldsymbol{x} \in \partial\Omega^2, t > 0)$$
$$(\boldsymbol{V}C - \boldsymbol{D}.\nabla C)\boldsymbol{\eta}_{\partial\Omega} = g_3(\boldsymbol{x},t), \quad (\boldsymbol{x} \in \partial\Omega^3, t > 0)$$

where Ω is a domain of $\mathbb{R}^2$; $\partial\Omega^1, \partial\Omega^2$ and $\partial\Omega^3$ are partitions of the boundary $\partial\Omega$ of Ω corresponding to Dirichlet, Neumann and total flux boundary conditions; and $\boldsymbol{\eta}_{\partial\Omega}$ is the unit outward vector normal to the boundary $\partial\Omega$.

Classical Eulerian methods such as finite differences or finite elements are not suitable for the solution of the transport equation. Indeed, these methods can generate numerical solutions with artificial diffusion and/or non-physical oscillations when advection is dominant[3]. Very fine spatial and temporal discretizations can be used to improve the quality of the results but at the cost of an important computational effort.

Because of the hyperbolic nature of advection, characteristic analysis is natural to aid in the solution of equation (1) and has led to many related approximation techniques including Eulerian-Lagrangian methods (ELM) and method of characteristics (MOC)[4]. With these methods the advective component is treated by a characteristic tracking algorithm and the diffusive step is treated separately using an Eulerian approximation. Therefore, the Courant number limitation of purely Eulerian methods is avoided because of the Lagrangian treatment of advection[1]. However, these methods fail to conserve mass and are unable to rigorously treat boundary conditions[5].

The Eulerian-Lagrangian localized adjoint method was developed about 20 years ago by Celia *et al.*[1]. The ELLAM is an improved characteristic method which uses space-time test functions. The method conserves mass and treats general boundary conditions naturally in its formulation. A review of the researches done on the ELLAM is given by Russell and Celia[6].

Many formulations of the ELLAM were developed during last years (Healy and Russell[5], Russell and Celia[6], Binning and Celia[7], Younes[8], Younes and Ackerer[2])
Almost all developed ELLAMs suffer from non-physical oscillations and/or numerical dispersion. Indeed, for unstructured meshes, oscillations can appear because quadrature weights (defined at the old time level) will not necessary sum up to the correct volume for each mesh element at the new time level. This phenomenon can be minimized by using Strategic Space Integration Points (SSIP) coupled with the backtracking approach[5]. Furthermore, it is also known that Eulerian-Lagrangian methods perform well for problems in which they can successfully use a large time step but they can suffer from numerical dispersion introduced by interpolation at each time step when the method is used with several time steps[9].

To overcome these difficulties, a new formulation of the ELLAM was developed by Younes *et al.*[2] to solve the Advection Dispersion transport Equation (ADE) on unstructured triangular meshes. The new scheme requires a very limited number of integration points (usually one per element) even for unstructured meshes. With this scheme, only strategic integration points are used as numerical integration points. Location of strategic integration points and weights are assigned at the new time level and then backtracked to the old time level without redistributing the weights. In order to avoid excessive numerical diffusion when dealing with

several time steps, continuous characteristics are used and only changes due to dispersion are interpolated to obtain the concentration at the foot of each characteristic.
In the following, we show applicability and efficiency of this scheme for highly heterogeneous domains including injection and pumping wells.

2 THE NEW ELLAM FORMULATION FOR ADE

The weak formulation of equation (1) using space-time function $\omega(x,t)$ leads to:

$$\int_0^T \int_\Omega \left[\frac{\partial C}{\partial t}\omega + \nabla.(\boldsymbol{V}C)\omega - \nabla.(\boldsymbol{D}.\nabla C)\omega \right] dxdt = 0 \tag{4}$$

$\omega(x,t)$ is defined for $t \in \left[t^n, t^{n+1} \right]$ and verifies the local adjoint equation:

$$\frac{D\omega}{Dt} = \frac{\partial \omega}{\partial t} + \boldsymbol{V}.\nabla \omega = 0 \tag{5}$$

Therefore, the ADE to solve becomes (for details, see[7])

$$\int_\Omega C^{n+1}\omega^{n+1}(x)dx + \int_0^T \int_\Omega (\boldsymbol{D}.\nabla C)\nabla \omega dxdt + \int_0^T \int_{\partial\Omega} \left[(\boldsymbol{V}C - \boldsymbol{D}.\nabla C)\omega \right] \boldsymbol{n}_{\partial\Omega} dxdt = \int_\Omega C^n \omega^n(x)dx \tag{6}$$

Terms of this equation correspond respectively to the mass concentration at the new time level $(n+1)$, the dispersion exchange, the mass concentration entering or leaving the domain from boundaries and the mass concentration at the old time level (n).
The main difficulty of ELLAM is the evaluation of the mass concentration at the old time level (n). This term is approximated with a numerical quadrature using N_E integration points with their corresponding space weights W_E^p:

$$\int_\Omega C^n \omega^n(x)dx = \sum_E \left[\sum_{p=1}^{N_E} (C^n(x^p,t^n)\omega(x^p,t^n)W_E^p \right] \tag{7}$$

The integration points are located at x^p at time t^n and tracked forward to $\overline{x^p}$ at t^{n+1} to evaluate $\omega(x^p,t^n) = \omega(\overline{x^p},t^{n+1})$ or tracked backward from x^p at time t^{n+1} to $\overline{x^p}$ at t^n to find $\omega(x^p,t^{n+1}) = \omega(\overline{x^p},t^n)$. The concentration $C^n(x^p,t^n)$ is evaluated by linear interpolation of the known solution at the nodes of the mesh.

The ELLAM formulation developed by Younes *et al.*[2] requires the following three stages:

a- First, we place P integration points strategically in the centre of all elements at each time level. The weights W^P correspond to the area of each element. Then, each particle is tracked backward from its position x_{fin}^p at t^{n+1} to the departure position x_{in}^p at time $t=0$ or until we reach the boundary of the domain. Here, we can differentiate particles entering the domain from the boundary $(t \neq 0)$ and particles which are initially located inside the domain $(t=0)$.

b- Initial concentration of all particles located inside the domain (with $t=0$) are evaluated by interpolating the known concentrations at the nodes of the mesh. Then, particles are tracked forward to the next time level. Only particles which arrives at the centre of

elements are used to obtain the solution of the equation (6). This gives us the new concentration $C_i^{adv+disp}$ by advection and dispersion at each node i of the mesh.

c- The third step consists in updating particle's concentration C_p^{new} which serves to calculate the concentration for the following times steps. In this purpose, we interpolate only the change by dispersion in order to reduce numerical dispersion introduced by interpolation as shown by Younes *et al.*[10]

To take into account sink and source terms for the transport problem, cells containing the injection (respectively the pumping) well should be small enough to have only outflow (respectively inflow) at all cell edges. In this case, the boundaries of the cell containing the well are considered as the boundaries of the domain for the transport simulation. The particles which cross these edges during backtracking are considered as boundary integration points.

This ELLAM formulation is compared to the Galerkin Discontinuous Finite Element Method (DFEM) for transport problems on highly heterogeneous domains.

3 NUMERICAL EXPERIMENTS

a- Test case 1:

The spatial domain Ω is a unit square with sand (blue) and clay (red) as shown in figure 1. 18000 triangular elements are used for the spatial discretization. A flux of $Q_{in} = -1.10^{-1}\text{m.day}^{-1}$ is prescribed at the left lower corner and a flux of $Q_{out} = 1.10^{-1}\text{m.day}^{-1}$ in the upper right corner. The stationary flow problem is solved with the lumped mixed finite element method[11], the velocity is defined everywhere in the field and is continuous across the inter-element boundaries. The pressure distribution and the velocity field are shown in figure 2.

The boundary conditions for the transport problem are of Dirichlet type at the inflow (left lower corner) $\begin{cases} C = 1\ \text{mg.L}^{-1} \text{ for } x = 0 \text{ and } y < 0.015 \\ C = 1\ \text{mg.L}^{-1} \text{ for } x < 0.015 \text{ and } y = 0 \end{cases}$ (8)

The dispersion parameters are: $\alpha_L^{sand} = 2.10^{-2}\text{m}$, $\alpha_T^{sand} = 2.10^{-3}\text{m}$ for the sand and for the clay $\alpha_L^{clay} = 2.10^{-4}\text{m}$, $\alpha_T^{clay} = 2.10^{-5}\text{m}$. The molecular diffusion is fixed to $3{,}6.10^{-10}\text{m}^2\text{.day}^{-1}$.

Simulations are performed for a final time of 2,5 days. The CPU_times as well as the maximum and the minimum values of obtained concentrations with ELLAM and DFEM are shown in Table-1.

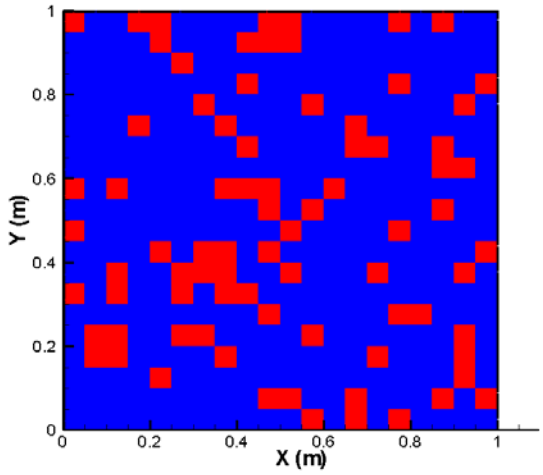

Figure 1: Domain with sand and clay

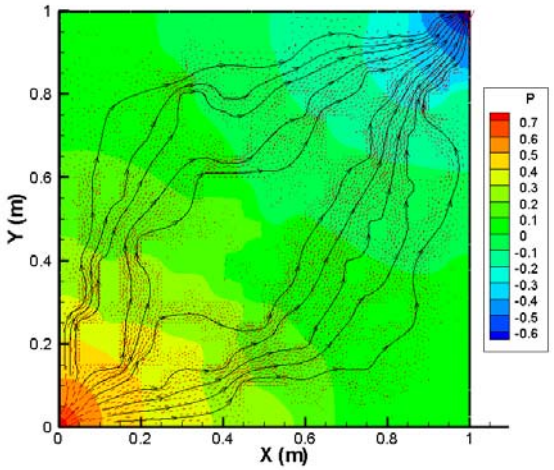

Figure 2: Pressure and velocity fields

METHOD	ELLAM	DFEM
CPU_time (s)	4.796	101.42
Max concentration ($mg.L^{-1}$)	1.0	1.0
Min concentration ($mg.L^{-1}$)	0	0

Table-1: Results of ELLAM and DFEM for case-1

The results show that the DFEM requires much more computational time than the ELLAM. Indeed, contrarily to ELLAM, the DFEM requires small time steps to fulfil the CFL constraint.

Obtained results with both methods are visualized in figures 3 and 4.

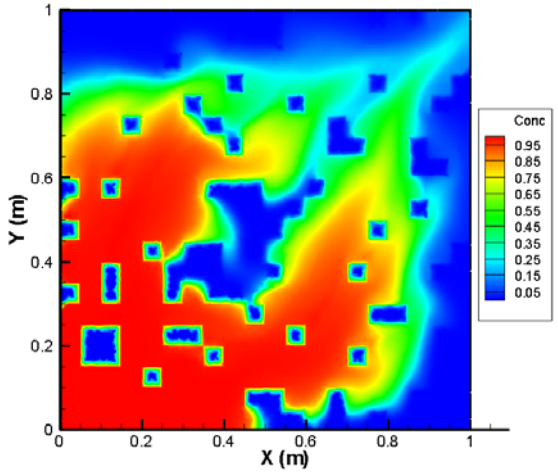

Figure 3: Concentration obtained with New_ELLAM

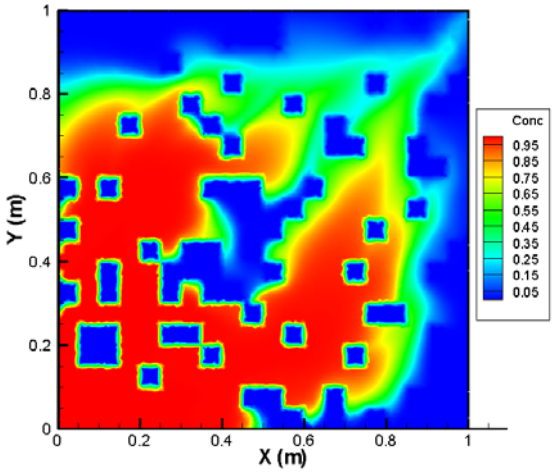

Figure 4: Concentration obtained with DFEM

b- Test case 2:

The second test case is a highly heterogeneous domain (sand and clay) with injection and pumping wells. The spatial domain Ω has a rectangular shape $(0,140)\times(0,70)$ which is partitioned into 10000 triangular elements (figure 5). The values of the flow rate in the injection and the pumping wells are $Q_{inj} = -Q_{pump} = 5\text{m}^3.\text{day}^{-1}$. A fixed head $h_{left} = 15$ m is imposed at the left boundary of the domain and $h_{right} = 0$ m at the right boundary. The flow equation is solved with the mixed finite element method (figure 6). Transport results obtained with both methods are given in table 2.

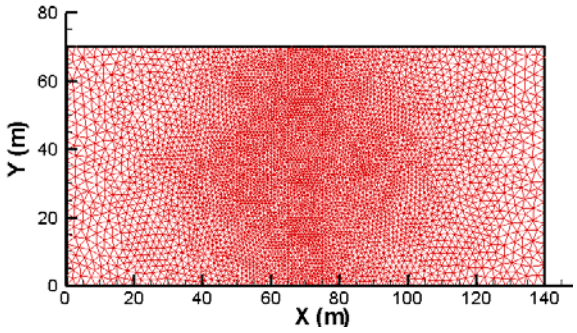

Figure 5: Domain discretized with triangular element

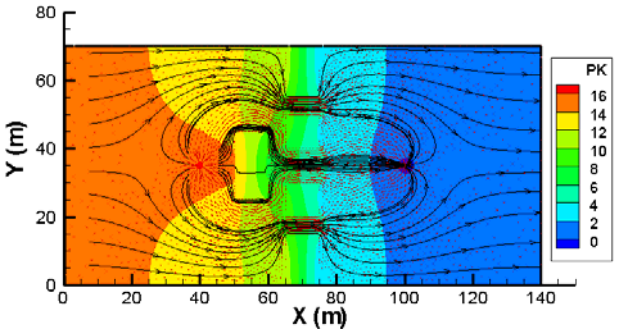

Figure 6: Pressure and velocity field

A fixed concentration of $C = 1\text{mg.L}^{-1}$ is prescribed at the injection well during 800 days. The dispersion parameters are similar to case 1.

METHOD	ELLAM	DFEM
CPU_time (s)	27.68	104.68
Max concentration (mg.L^{-1})	1.0	1.0
Min concentration (mg.L^{-1})	0	0

Table-2: Comparison of acquired results for case-2

The concentration distributions obtained with both methods are shown in figures 7 and 8.

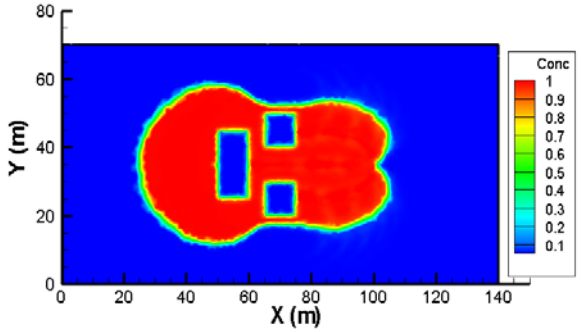

Figure 7: Concentration obtained with New_ELLAM

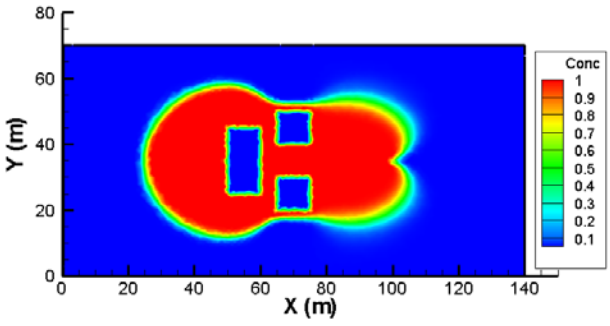

Figure 8: Concentration obtained with DFEM

Similar results are obtained. As previously, the DFEM is less efficient than the ELLAM. The ELLAM formulation is able to treat accurately general problems on heterogeneous domains with sink/source terms.

4 CONCLUSIONS AND PERSPECTIVES

The ELLAM is used on triangular meshes and highly heterogeneous domains with injection and pumping wells. The ELLAM formulation appears to be accurate and very efficient since it can be used with large time steps. The number of integration points is very limited and unphysical oscillations are avoided.

The next step of this work is to combine the ELLAM formulation with the Sequential Non Iterative Approach to solve advective-diffusive-reactive transport equation with biodegradation.

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