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A Nonoverlapping Characteristic Domain Decomposition Method for Unsteady State Advection-Diffusion Equations

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Introduction

Advection-diffusion partial differential equations (PDEs) arise in petroleum reservoir simulation, subsurface contaminant transport and remediation, and many other applications. These problems typically exhibit solutions with moving steep fronts within some relatively small regions, where important chemistry and physics take place. Furthermore, an identifying feature of these applications is the presence of extremely large scale fluid flows coupled with transient transport of physical quantities such as pollutants, chemical species, radionuclides, and temperature. Consequently, an extremely refined global mesh is not feasible due to the excessive computational and storage cost. Domain decomposition techniques prove to be a feasible and powerful approach for the solution of these problems, because they allow a significant reduction of the size of the problems and the use of different physical or numerical models on different subdomains to model fluid flows more accurately. Furthermore, they are easily parallelizable.

However, many domain decomposition methods that work well for elliptic and

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parabolic PDEs [SBG96] can perform very poorly for advection-diffusion PDEs. For example, the well known Dirichlet-Neumann algorithm [BW86, MQ89], which assigns a Dirichlet condition to one subdomain and a Neumann boundary condition to its adjacent subdomain, and has been successfully applied to solve diffusion dominated problems, could generate nonphysical layers at each iteration. The fundamental reason is that these methods do not necessarily take into account the advection dominance or the hyperbolic nature of advection-diffusion PDEs. In particular, even though the Dirichlet-Neumann matching conditions are mathematically correct, they might not respect the hyperbolic limit of advection-diffusion problems. The errors generated at subdomain interfaces are then propagated into the interior domain and could destroy the accuracy of the solutions on the entire domain.

Extensive research has been carried out on developing domain decomposition methods for advection-diffusion problems. Cai [Cai91, Cai94] developed multilevel additive and multiplicative Schwarz preconditioners for parabolic and unsteady state advection-diffusion PDEs. On the other hand, the Adaptive Dirichlet Neumann (ADN) and Adaptive Robin Neumann (ARN) nonoverlapping domain decomposition methods introduced in [GGQ96, Cic96, Tro96] choose interface conditions to be adapted to the local flow direction. These methods prevent the rise of artificial layers at subdomain interfaces as the advection becomes dominant. While these methods could solve the discrete algebraic systems with strongly nonsymmetric coefficient matrices fairly efficiently at each time step, the underlying numerical methods used in these domain decomposition algorithms are standard finite element/difference/volume methods or upwinding methods with temporal discretization in time. It is well known that standard finite element/difference/volume methods tend to generate solutions with serious non-physical oscillations while upwinding methods often produce solutions with excessive numerical dispersion and grid orientation effect when applied for solving time-dependent advection-diffusion PDEs, unless the spatial grids and time steps are chosen small enough such that the mesh Peclet number is around one and the Courant number is less than or equal to one [CRHE90, WALT97, WDEESM].

Characteristic methods (e.g. the modified method of characteristics by Douglas and Russell [DR82]) effectively solve the advective component by a characteristic tracking algorithm and treat the diffusive term separately. These methods symmetrize the governing PDEs and generate accurate numerical solutions even if large time steps are used. Unfortunately, many characteristic methods fail to conserve mass and have difficulty in treating boundary fluxes when characteristics intersect the boundary of the domain. This is one of the reasons why the few characteristic domain decomposition methods developed so far are overlapping domain decomposition methods [TJDE97]. The Eulerian-Lagrangian localized adjoint method (ELLAM), which was first presented in [CRHE90] by Celia, Russell, Herrera, and Ewing, provides a general characteristic solution procedure for the solution of advection-diffusion PDEs with general boundary conditions in a mass conservative manner. Thus, ELLAM overcomes the principle shortcomings of previous characteristic methods while maintaining their numerical advantages. Our previous work [WALT97, WDEESM] also show that ELLAM schemes generate accurate solutions even if very large time steps and spatial grids are used, and often outperform many well received and widely used numerical methods.

In this paper we present an ELLAM-based, nonoverlapping characteristic domain decomposition method for unsteady state advection-diffusion equations. With the standard Dirichlet-Neumann interface condition, with which many domain decomposition methods are known to generate poor solutions for advection-diffusion PDEs, our domain decomposition method produces accurate and stable solutions that are free of artifacts even if large time steps are used in the simulation. Numerical experiments are presented to show the strong potential of the method.

An Underlying Numerical Method

In this section we briefly outline an underlying Runge-Kutta Eulerian-Lagrangian localized adjoint method (RKELLAM) [WALT97, WDEESM] for the model problem

$$u_t + (V(x,t)u - D(x,t)u_x)_x \;=\; f(x,t) \qquad x \in (a,b),\ t \in (0,T], \tag{1}$$

with an initial condition and any combination of Dirichlet, Neumann, or flux boundary conditions at the two boundary points $x = a$ and $x = b$. $V(x,t)$ is the velocity field and $D(x,t)$ is the diffusion coefficient, both of which are assumed positive.

Let I and N be two positive integers, we define a space-time partition: $x_i = a + i\Delta x$ $(0 \leq i \leq I)$ with $\Delta x = (b-a)/I$ and $t_n = n\Delta t$ $(0 \leq n \leq N)$ with $\Delta t = T/N$. Multiplying Eq. (1) by a test function w that vanishes outside $[a,b] \times (t^n, t^{n+1}]$ and integrating the resulting equation by parts we obtain

$$\begin{aligned} &\int_a^b u(x,t^{n+1})w(x,t^{n+1})\,dx + \int_{t^n}^{t^{n+1}} \int_a^b D u_x w_x \,dxdt \\ &\qquad + \int_{t^n}^{t^{n+1}} (Vu - Du_x)w\Big|_a^b \,dt - \int_{t^n}^{t^{n+1}} \int_a^b u(w_t + V w_x)\,dxdt \\ &= \int_a^b u(x,t^n)w(x,t^n_+)\,dx + \int_{t^n}^{t^{n+1}} \int_a^b f w \,dxdt, \end{aligned} \tag{2}$$

where $w(x,t^n_+) = \lim_{t\to t^n_+} w(x,t)$, which takes into account the fact that $w(x,t)$ is discontinuous in time at time t^n.

Based on the weak form (2), we derive a RKELLAM scheme through the following steps: (i) We approximate the characteristic curves of Eq. (1) by a second-order Runge-Kutta approximation. (ii) We define the test functions w to be the standard hat functions on $[a,b]$ at time t^{n+1} and at the outflow boundary $\{b\} \times [t^n, t^{n+1}]$, and extend w constant along the characteristics into the space-time strip $[a,b] \times [t^n, t^{n+1}]$. (iii) We incorporate these test functions into the weak form (2) and evaluate the temporal integrals in the second terms on both sides of Eq. (2) by the trapezoidal quadrature along the characteristics, leading to terms defined on $[a,b]$ at the time levels t^n and t^{n+1} as well as on the outflow boundary $\{b\} \times [t^n, t^{n+1}]$. (iv) We incorporate the inflow and outflow boundary conditions into the third term on the left-hand side of weak form (2). (v) We approximate the solution u in Eq. (2) by a piecewise linear trial function on $[a,b]$ at time t^{n+1} and at the outflow boundary $\{b\} \times [t^n, t^{n+1}]$. (vi) The last (adjoint) term on the left-hand side of Eq. (2) is dropped since it only measures the error of characteristic tracking which is within the desired order.

With the prescribed inflow and outflow boundary conditions as well as the solution $u(x,t^n)$ which is known from the computations at the previous time level, the derived

RKELLAM scheme solves for $u(x, t^{n+1})$ and $u(b, t)$ for $t \in [t^n, t^{n+1}]$. The RKELLAM scheme also symmetrizes the governing equation (1), generates accurate numerical solutions even if large time steps are used, and conserves mass. Due to the length constraint, we omit the detailed derivation of the RKELLAM scheme. We refer readers to [WALT97, WDEESM] for details of RKELLAM and for its comparison with many well received and widely used methods that shows the strength of this method.

A Nonoverlapping Characteristic Domain Decomposition Method

In this section we derive a nonoverlapping characteristic domain decomposition method for the model problem (1), based on the RKELLAM scheme in the previous section. We choose the standard Dirichlet-Neumann matching condition at subdomain interfaces, despite that many domain decomposition methods with the Dirichlet-Neumann matching condition generate poor solutions for advection-diffusion PDEs. The numerical experiments in the next section show that our method generates accurate and stable solutions that are free of artifacts. This is due to the fact that the underlying RKELLAM scheme symmetrizes the governing equation (1). In other words, the governing equation (1) can be written as a parabolic equation without any advective term along the characteristics. This is why our method is free of the problems other methods suffer from. The detailed method is described below

Partition of the Domain

Decompose the spatial domain $\Omega = [a, b]$ into a union of $2M$ subdomains

$$\Omega = \bigcup_{i=1}^{2M} \Omega^{(i)}, \qquad \Omega^{(i)} = [d_{i-1}, d_i], \quad i = 1, 2, \ldots, 2M \tag{3}$$

with

$$a = d_0 < d_1 < d_2 < \ldots < d_{2M} = b. \tag{4}$$

for $n = 0, 1, \ldots, N-1$ **do**

Initialize the iteration parameter $l = 0$.
if Error > Tolerance **then**
$l = l + 1$.

L1. **for** $i = 1, 3, \ldots, 2M-1$ **do**

A. Use the prescribed inflow boundary condition at $x = a$ for $\Omega^{(1)}$ and the following relation

$$u^{(l)}(d_{i-1}^{+}, t) = u^{(l-1)}(d_{i-1}^{-}, t), \qquad i = 3, 5, \ldots, 2M-1 \tag{5}$$

to define an artificial inflow Dirichlet boundary condition for the subdomain $\Omega^{(i)}$ ($i = 3, 5, \ldots, 2M-1$). Here $u(d_{i-1}^{-}, t)$ and

$u(d_{i-1}^{+},t)$ represent the left- and right-limits of u at the point d_{i-1}, respectively, and $u^{(0)}(d_{i-1}^{-},t)$ is defined by

$$u^{(0)}(d_{i-1}^{-},t) = u(d_{i-1}^{*}(t),t^{n}), \qquad i = 3,5,\ldots,2M-1, \tag{6}$$

where $d_{i-1}^{*}(t) \in \Omega^{(i-1)}$ is the point at time level t^n which the point (d_{i-1},t) backtracks to.

B. Use the relation

$$u_x^{(l)}(d_i^{-},t) = u_x^{(l-1)}(d_i^{+},t), \qquad i = 1,3,\ldots,2M-1 \tag{7}$$

to define an artificial outflow Neumann boundary condition for the subdomain $\Omega^{(i)}$ $(i = 1,3,\ldots,2M-1)$. Here $u_x^{(0)}(d_i^{+},t)$ is defined by

$$u_x^{(0)}(d_i^{+},t) = u_x(d_i^{*}(t),t^{n}), \qquad i = 1,3,\ldots,2M-1, \tag{8}$$

where $d_i^{*}(t) \in \Omega^{(i)}$ is the point at time level t^n which the point (d_i,t) backtracks to.

C. With the inflow and outflow boundary conditions introduced in Steps L1.A and L1.B, use the RKELLAM scheme presented in Section 17 to solve equation (1) on the *odd numbered* subdomains $\Omega^{(i)}$ $(i = 1,3,\ldots,2M-1)$ in parallel, yielding the l-th iterative solution $u^{(l)}(x,t^{n+1})$ on $\Omega^{(i)}$ and $u^{(l)}(d_i^{-},t)$ on the outflow boundary of $\Omega^{(i)}$ for all the *odd numbered* subdomains $\Omega^{(i)}$ $(i = 1,3,\ldots,2M-1)$.

end

L2. **for** $i = 2,4,\ldots,2M$ **do**

A. Use the following relation

$$u^{(l)}(d_{i-1}^{+},t) = u^{(l)}(d_{i-1}^{-},t), \qquad i = 2,4,\ldots,2M \tag{9}$$

to define an artificial inflow Dirichlet boundary condition for the subdomain $\Omega^{(i)}$ $(i = 2,4,\ldots,2M)$.

B. Use the prescribed outflow boundary condition at $x = b$ for the subdomain $\Omega^{(2M)}$ and the relation

$$u_x^{(l)}(d_i^{-},t) = u_x^{(l)}(d_i^{+},t), \qquad i = 2,4,\ldots,2M-2 \tag{10}$$

to define an artificial outflow Neumann boundary condition for the subdomain $\Omega^{(i)}$ $(i = 2,4,\ldots,2M-2)$. Here

$$\begin{aligned} u_x^{(l)}(d_i^{+},t) &= u_x(d_i^{*}(t),t^{n})\frac{t^{n+1}-t}{\Delta t} \\ &\quad + u_x^{(l)}(d_i^{**}(t),t^{n+1})\frac{t-t^{n}}{\Delta t}, \end{aligned} \tag{11}$$

where $d_i^{**}(t) \in \Omega^{(i+1)}$ is the point at time level t^{n+1} which the point (d_i,t) tracks forward to.

C. With the inflow and outflow boundary conditions introduced in Steps L2.A and L2.B, use the RKELLAM scheme presented in Section 17 to solve equation (1) on the *even numbered* subdomains $\Omega^{(i)}$ $(i = 2, 4, \ldots, 2M)$ in parallel, yielding the l-th iterative solution $u^{(l)}(x, t^{n+1})$ on $\Omega^{(i)}$ and $u^{(l)}(d_i^-, t)$ on the outflow boundary of $\Omega^{(i)}$ for all the *even numbered* subdomains $\Omega^{(i)}$ $(i = 2, 4, \ldots, 2M)$.

end

else

Define $u(x, t^{n+1}) = u^{(l)}(x, t^{n+1})$ on $\Omega^{(i)}$ for $i = 1, 2, \ldots, 2M$.

endif

end

Numerical Experiments

In this section we apply the domain decomposition method to two standard test problems to observe the performance of the method developed.

Example 1. This example considers the transport of a Gaussian pulse in a variable velocity field given by $V(x,t) = 1 + 0.01x$, the diffusion coefficient is $D(x,t) = 10^{-4}$. The spatial domain is $[a,b] = [0, 3.2]$. The initial Gaussian pulse is located at the inflow boundary $x = 0$, with a unit height and a spread or standard deviation of $\sigma = 0.0316$. In the experiments, six subdomains are used (i.e. $M = 3$)

$$[0, 3.2] = [0, 0.5] \cup [0.5, 1] \cup [1, 1.5] \cup [1.5, 2] \cup [2, 2.5] \cup [2.5, 3.2]. \tag{12}$$

$\Delta x = 0.01$ and $\Delta t = 0.02$. In the numerical experiments, four iterations are used. In Figure 1(A), the numerical solution is presented against the analytical solution at time instant $t = 0.5, 1, 1.5, 2$, and 2.5, when the numerical solution is located at the interfaces. The L_2 and L_1 norms of the absolute error at $t = 2.5$ are 4.53×10^{-4} and 1.92×10^{-4}, respectively.

Example 2. This example considers the transport of a diffused step function. All the parameters are the same as those in Example 1 with the only exception that the velocity field is $V(x,t) = 1$. The initial configuration is a box function of a unit height supported on the interval $[0.1, 0.4]$. The numerical solution is presented in Figure 1(B). The L_2 and L_1 norms of the absolute error at $t = 2.5$ are 1.33×10^{-3} and 5.80×10^{-4}, respectively.

Conclusion

In this paper we develop a nonoverlapping characteristic domain decomposition method for the solution of advection-diffusion equations, using the standard Dirichlet-Neumann matching conditions at subdomain interfaces. The numerical results show that the developed method generate accurate and stable solutions without noticeable artifacts even if large time steps are used, leading to greatly improved efficiency.

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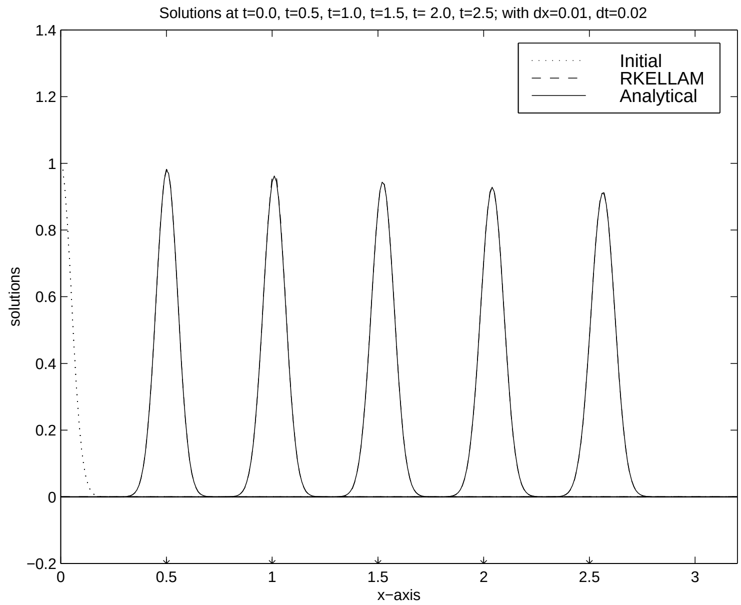
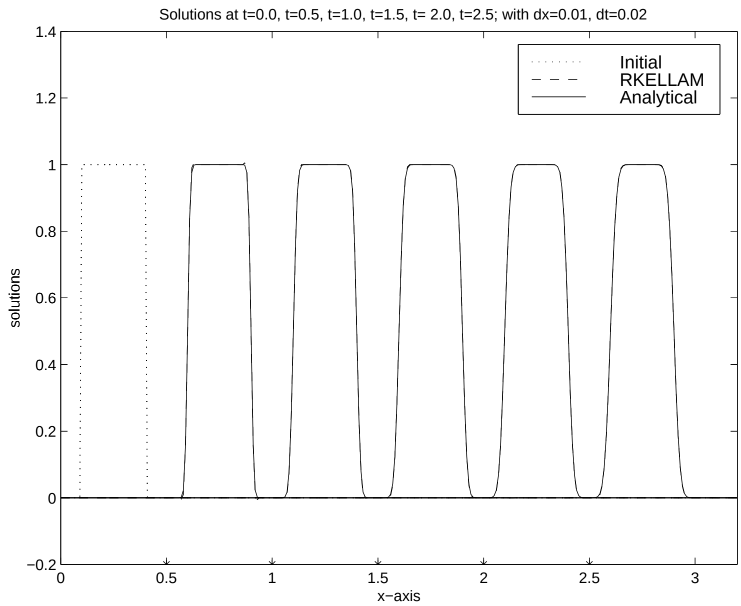


(A) Solutions of Example 1



(B) Solutions of Example 2

Figure 1 Solutions at time instance t= 0 (initial), 0.5, 1, 1.5, 2, 2.5