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AN EULERIAN LAGRANGIAN LOCALIZED ADJOINT METHODS FOR THE SOLUTION OF THE TRANSIENT ADVECTION DIFFUSION EQUATIONS IN THREE SPACE DIMENSIONS

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Abstract: We present a characteristic method for the solution of the transient advection diffusion equations in three space-dimensions. This method uses piecewise tri-linear trial and test functions over rectangular grids within the framework of the Eulerian Lagrangian localized adjoint methods (ELLAMs). It therefore maintains the advantages of previous ELLAM schemes. In particular, it treats general boundary conditions naturally in a systematic manner, conserves mass, and symmetrizes the governing transport equations. Moreover, it generates accurate numerical solutions even if large time steps are used in the simulation. Numerical experiments are presented to illustrate the performance of this method.

AMS Subject Classification: 65M25, 76M25, 35D99
Key Words: advection-diffusion equations, characteristic methods, Eulerian Lagrangian methods

1. Introduction

Advection-diffusion equations are a class of partial differential equations that are mathematically important because they arise in many problems in science and engineering. However, their importance also comes from the fact that they

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present serious numerical difficulties, especially when advection dominates the physical process. Standard finite difference and finite element methods, which are known to work well for many other types of equations, generate solutions for this class of equations that exhibit non-physical spurious oscillations and/or artificial numerical diffusion that smears out sharp fronts of the solutions where important chemistry and physics take place. A number of specialized methods have been proposed in the literature to resolve these difficulties. These methods generally are classified as *Eulerian methods* or *characteristic methods*. Eulerian methods, which are generally characterized by ease of formulation and implementation, use fixed spatial grids and incorporate some form of upstream weighing or some other dissipation technique in their formulations [3, 6, 9, 10, 13, 14]. Thus, they can eliminate the non-physical oscillations present in the standard finite difference and finite element methods. Some of these Eulerian methods, such as the Godunov schemes, the total variation diminishing (TVD) schemes, and the essentially and weighted essentially non-oscillatory (ENO and WENO) schemes, can resolve shock discontinuities from nonlinear hyperbolic conservation laws. Characteristic methods, on the other hand, make use of the hyperbolic nature of the governing equation by utilizing tracking along the characteristics to treat the advective part of the governing equation [7, 11]. These methods symmetrize the governing equations and significantly reduce the temporal truncation errors when compared to Eulerian methods. Thus, they allow large time steps to be used in the numerical simulations without any sacrifice in accuracy, and leads to a greatly improved efficiency. However, most characteristic methods have difficulties in treating general boundary conditions and fail to conserve mass.

The Eulerian Lagrangian localized adjoint method (ELLAM) was proposed by Celia, Russell, Herrera, and Ewing [5] as an alternative characteristic formulation that alleviates the difficulties mentioned. This ELLAM formalism provides a general characteristic solution procedure for advection-diffusion equations and a consistent framework for conserving mass and treating general boundary conditions. The original ELLAM method is for the solution of one dimensional constant-coefficient advection-diffusion equations, in which piecewise-linear trial and test functions are used in the weak formulation. The strong potential of this method leads to the development of two- and three-dimensional ELLAM schemes using either the finite element or finite volume approaches [2, 8, 16]. Motivated by the success of these ELLAM schemes, we present in this paper an ELLAM method for the solution of the transient advection-diffusion equation in three space dimensions. This method uses piecewise tri-linear test and trial functions over rectangular prism finite elements (bricks). The characteristics tracking can be achieved by any of first-order Euler, second-order Runge-Kutta, or fourth-order Runge-Kutta algorithms. Numerical experiments are presented to illustrate the performance of the scheme developed.

2. Development of the ELLAM Schemes

We consider the following three-dimensional transient advection diffusion equation

$$(\phi(\mathbf{x},t)\, u(\mathbf{x},t))_t + \nabla \cdot \Big(\mathbf{v}(\mathbf{x},t)u(\mathbf{x},t) - \mathbf{D}(\mathbf{x},t)\nabla u(\mathbf{x},t)\Big) = f(\mathbf{x},t)\,, \qquad (1)$$

where $\mathbf{x} = (x,y,z)$, $u_t = \partial u/\partial t$, $\nabla = \langle \partial/\partial x, \partial/\partial y, \partial/\partial z \rangle$, $\phi(\mathbf{x},t)$ is the retardation coefficient, $\mathbf{v}(\mathbf{x},t)$ is the velocity field, $\mathbf{D}(\mathbf{x},t)$ is the diffusion-dispersion tensor, and $f(\mathbf{x},t)$ is a source/sink term. While the ELLAM method can be developed for any bounded spatial domain which admits a quasi-uniform triangulation, for simplicity of presentation we consider a spatial domain of the form $\Omega = [a,b] \times [c,d] \times [g,h]$. To close the system, we assume that an appropriate initial condition and any proper combination of Dirichlet, Neumann, or flux boundary conditions are specified at the inflow or outflow parts of the boundary.

2.1. Partition and Characteristic Tracking

The ELLAM methods can be developed for any quasi-uniform partition of the space-time domain $\Omega \times [0,T]$. However, for simplicity of presentation, we consider the following uniform rectangular partition

$$\begin{array}{lll} x_i = a + i\,\Delta x & i = 0,\ ...,\ I & \text{with}\ \ \Delta x = (b-a)/I\,, \\ y_j = c + j\,\Delta y & j = 0,\ ...,\ J & \text{with}\ \ \Delta y = (d-c)/J\,, \\ z_k = g + k\,\Delta z & k = 0,\ ...,\ K & \text{with}\ \ \Delta z = (h-g)/K\,, \\ t^n = n\,\Delta t & n = 0,\ ...,\ N & \text{with}\ \ \Delta t = T/N\,, \end{array} \qquad (2)$$

where I, J, K, and N are positive integers. In the numerical formulation, we use a time-stepping procedure. Hence, we only need to focus on the current time interval $(t^{n-1}, t^n]$. By multiplying equation (1) by a piecewise smooth test function w that vanishes outside $\Omega \times (t^{n-1}, t^n]$ we obtain a weak form of equation (1)

$$\int_\Omega (\phi\, u)(\mathbf{x}, t^n)\; w(\mathbf{x}, t^n)\; d\mathbf{x} + \int_{t^{n-1}}^{t^n} \int_\Omega (\mathbf{D}\nabla u)\cdot \nabla w\; d\mathbf{x}\; dt$$
$$- \int_{t^{n-1}}^{t^n} \int_\Omega u(\phi\, w_t + \mathbf{v}\cdot\nabla w)\; d\mathbf{x}\; dt + \int_{t^{n-1}}^{t^n} \int_{\partial\Omega} (\mathbf{v}\, u - \mathbf{D}\nabla u)\; w\cdot \mathbf{n}\; dS$$
$$= \int_\Omega (\phi\, u)(\mathbf{x}, t^{n-1})\; w(\mathbf{x}, {t^{n-1}}_+)\; d\mathbf{x} + \int_{t^{n-1}}^{t^n} \int_\Omega f\; w\; d\mathbf{x}\; dt\,, \quad (3)$$

where $w(\mathbf{x}, {t^{n-1}}_+) = \lim_{t\to {t^{n-1}}^+} w(\mathbf{x}, t)$ which takes into account the fact that w is discontinuous in time at time t^{n-1}.

In the ELLAM framework [5], the test functions $w(\mathbf{x}, t)$ in equation (3) are selected to satisfy, within the tolerance of the accuracy desired, the homogeneous equation of the hyperbolic part of the adjoint equation of (1)

$$\phi\, w_t + \mathbf{v}\cdot\nabla w = 0 \quad (4)$$

to reflect the Lagrangian nature of equation (1), in other words, the test functions should be chosen to be constant along the characteristics. These characteristic curves of equation (1) are defined as solutions to initial value problems for the ordinary differential equation

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}_\phi(\mathbf{x}, t) := \left(\frac{\mathbf{v}(\mathbf{x}, t)}{\phi(\mathbf{x}, t)}\right). \quad (5)$$

However, solving this equation for a generic velocity field is not possible, in general. Thus, we need to use some numerical means to track the characteristics approximately. A variety of algorithms may be used for that purpose, including the Euler and Runge-Kutta methods. In our formulation, we use a second-order Runge-Kutta method (Heun method) and define the approximate characteristic curve $X(\theta; \bar{\mathbf{x}}, \bar{t})$ emanating from a point $(\bar{\mathbf{x}}, \bar{t})$ with $t \in [t^{n-1}, t^n]$ by

$$X(\theta; \bar{\mathbf{x}}, \bar{t}) = \bar{\mathbf{x}} + \frac{\theta - \bar{t}}{2}\Big(\mathbf{v}_\phi(\bar{\mathbf{x}}, \bar{t}) + \mathbf{v}_\phi(\bar{\mathbf{x}} - (\theta - t)\mathbf{v}_\phi(\bar{\mathbf{x}}, \bar{t}), \bar{t})\Big). \quad (6)$$

Here θ is the time position along that characteristic. Moreover, to further improve the accuracy of tracking, we subdivide the global step Δt into a number of micro time steps, and carry the tracking described by equation (6) across these micro steps.

2.2. The Reference Equation

The ELLAM method can be formulated by evaluating the space-time integrals in equation (3) along the approximate characteristics. Special attention needs to be given to the second (source and sink) term on the right-hand side of the equation and the second (diffusion) term on the left-hand side. These integrals, in a similar way to all other terms, are changed to the characteristic variables, and then a backward Euler quadrature along the characteristics is applied. This results in the following formulation for the ELLAM scheme

$$\begin{aligned}
&\int_\Omega \phi(\mathbf{x},t^n)\, u(\mathbf{x},t^n)\, w(\mathbf{x},t^n)\, d\mathbf{x} + \int_\Omega \Delta t^{(I)}(\mathbf{x})(\mathbf{D}\nabla u)(\mathbf{x},t^n)\cdot\nabla w(\mathbf{x},t^n)\, d\mathbf{x}\\
&\quad + \int_{t^{n-1}}^{t^n}\int_{\partial\Omega^{(O,n)}} \Delta t^{(O)}(\mathbf{x},t)\big((\mathbf{D}\nabla u)\cdot\nabla w\big)\,(\mathbf{v}\cdot\mathbf{n})\, dS\\
&\quad - \int_{t^{n-1}}^{t^n}\int_\Omega u\,(\phi\, w_t + \mathbf{v}\cdot\nabla w)\, d\mathbf{x}\, dt + \int_{t^{n-1}}^{t^n}\int_{\partial\Omega}(\mathbf{v}u - \mathbf{D}\nabla u)\cdot\mathbf{n}\, w\, dS\\
&= \int_\Omega \phi(\mathbf{x},t^{n-1})\, u(\mathbf{x},t^{n-1})\, w(\mathbf{x},{t^{n-1}}_+)\, d\mathbf{x} + \int_\Omega \Delta t^{(I)} f(\mathbf{x},t^n)\, w(\mathbf{x},t^n)\, d\mathbf{x}\\
&\quad + \int_{t^{n-1}}^{t^n}\int_{\partial\Omega^{(O,n)}} \Delta t^{(O)}(\mathbf{x},t) f\, w\,(\mathbf{v}\cdot\mathbf{n})\, dS + \mathcal{E}(u,w)\,, \qquad (7)
\end{aligned}$$

where $\partial\Omega^{(O,n)}$ is the outflow part of the boundary, $\mathcal{E}(u,w)$ is the truncation error due to the use of Euler quadrature, $\Delta t^{(I)}\mathbf{x} = t^n - t^*(\mathbf{x})$, where $t^*(\mathbf{x})$ is the time instance when the characteristic emanating from $(\mathbf{x}, t^n)$ intersects the boundary $\partial\Omega \times [t^{n-1}, t^n]$, and similarly $\Delta t^{(O)}(\mathbf{x},t) = t - t^*(\mathbf{x},t)$, where $t^*(\mathbf{x},t)$ is the time instance when the characteristic emanating from $(\mathbf{x},t)$ intersects the boundary; both time steps extend to Δt when the corresponding characteristics do not intersect the boundary.

3. Numerical Approximation

The numerical formulation of the ELLAM schemes can use arbitrarily high-order trial and test functions [1]. Here we present the scheme using piecewise tri-linear basis functions over rectangular brick elements determined by partition (2). The original one dimensional ELLAM scheme [5] uses the hat functions at time t^n

$$l_i(x,t^n) = \begin{cases} \dfrac{x - x_{i-1}}{\Delta x}, & \text{if } x \in [x_{i-1}, x_i]\,, \\ \dfrac{x_{i+1} - x}{\Delta x}, & \text{if } x \in [x_i, x_{i+1}]\,, \\ 0, & \text{otherwise}\,, \end{cases} \tag{8}$$

as basis functions (see Figure 1). The three dimensional ELLAM scheme is the natural extension which uses three-dimensional piecewise tri-linear polynomials that are formed by taking tensor products of associated one dimensional basis functions (8).

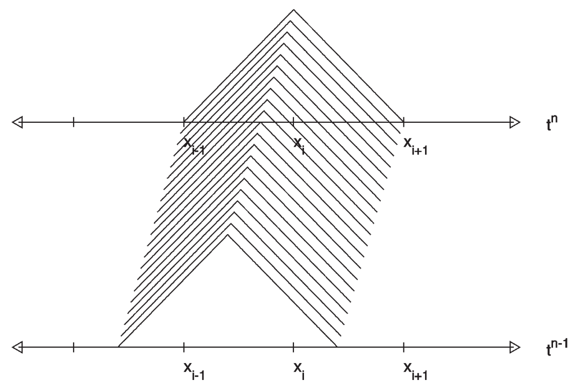


Figure 1: A basis function used in the original one-dimensional ELLAM scheme assuming a constant velocity

That is, if $l_i(x,t^n)$ is the piecewise linear function defined along x at the grid point x_i, and $l_j(y,t^n)$ and $l_k(z,t^n)$ are the corresponding functions along y at the grid point y_j and along z at the grid point z_k, respectively, then the piecewise tri-linear basis function associated with node m located at the grid point (x_i, y_j, z_k) is defined by $w_m(\mathbf{x},t^n) = l_i(x,t^n)\, l_j(y,t^n)\, l_k(z,t^n)$. The method uses similar basis functions at the outflow boundary of the space-time domain. Here we recall that in the interior of the domain, these test functions extend to be constant along the approximate characteristics.

The ELLAM scheme is based on approximating the exact solution u of equation (1) (or equivalently the reference equation (7)) by a piecewise tri-linear function U over the spatial partition (2). Incorporating the trial and test functions discussed above into the reference equation (7) and dropping the truncation error term $\mathcal{E}(u,w)$ and the adjoint term, the fourth term on the left side of the equation, gives the corresponding ELLAM scheme

$$
\begin{aligned}
&\int_\Omega \phi(\mathbf{x},t^n)\, U(\mathbf{x},t^n)\, w(\mathbf{x},t^n)\, d\mathbf{x} + \int_\Omega \Delta t^{(I)}(\mathbf{x})(\mathbf{D}\nabla U)(\mathbf{x},t^n)\cdot \nabla w(\mathbf{x},t^n)\, d\mathbf{x} \\
&\qquad + \int_{t^{n-1}}^{t^n} \int_{\partial\Omega^{(O,n)}} \Delta t^{(O)}(\mathbf{x},t)\big((\mathbf{D}\nabla U)\cdot\nabla w\big)\,(\mathbf{v}\cdot\mathbf{n})\, dS \\
&\qquad\qquad + \int_{t^{n-1}}^{t^n} \int_{\partial\Omega} (\mathbf{v}U - \mathbf{D}\nabla U)\cdot \mathbf{n}\, w\, dS \\
&= \int_\Omega \phi(\mathbf{x},t^{n-1})\, U(\mathbf{x},t^{n-1})\, w(\mathbf{x},{t^{n-1}}_+)\, d\mathbf{x} + \int_\Omega \Delta t^{(I)} f(\mathbf{x},t^n)\, w(\mathbf{x},t^n)\, d\mathbf{x} \\
&\qquad + \int_{t^{n-1}}^{t^n} \int_{\partial\Omega^{(O,n)}} \Delta t^{(O)}(\mathbf{x},t) f\, w\, (\mathbf{v}\cdot\mathbf{n})\, dS. \qquad (9)
\end{aligned}
$$

All integrals involved in the ELLAM formulation (9) are standard with the exception of the first integral on the right-hand side. While more than one approach may be used to evaluate this integral, leading to various schemes, the approach we use is forward tracking [12, 8, 16]. In this approach, we enforce the integration at time t^{n-1} using the fixed grid (2) on which $U(\mathbf{x},t^{n-1})$ is piecewise smooth. The integration is carried by a numerical quadrature algorithm, where the value of $w_m(\mathbf{x},t^{n-1})$ at each quadrature point is obtained by forward tracking the point to time level t^n, where the test function is piecwise tri-linear. This approach avoids the difficulties associated with distorted grids which appear in many other characteristic methods.

With the known solution $U(\mathbf{x},t^{n-1})$ from the computations at the previous time step t^{n-1} (or the initial condition) and the prescribed boundary conditions, the ELLAM method (9) solves for $U(\mathbf{x},t^n)$ with $\mathbf{x}$ in Ω and also for $U(\mathbf{x},t)$ for points in $\Omega^{(O,n)}$. This method symmetrizes the governing equation (1), generates accurate numerical solutions even if large time steps are used, and conserves mass [5].

4. Numerical Experiments

In this section we present results of several test runs we carry to observe the performance of ELLAM method using a number of test problems with known analytical solutions.

4.1. Transport Subject to a Rotational Velocity

In this first example, we consider the transport of an initial configuration subject to an advection-dominated equation (1) with a velocity field of $\mathbf{v} = \langle -4y, 4x, 1\rangle$ and a relatively small diffusion tensor of $\mathbf{D} = 0.0001\mathbf{I}_3$, where $\mathbf{I}_3$ is the 3×3 identity matrix. The effect of this rotational velocity field in the x and y directions is to cause the initial configuration to travel on a circular helical path around the z direction. The domain of the problem is $[-0.5, 0.5]^2 \times [0, 2]$ and we simulate for a time period of $[0, \pi/2]$.

For an initial condition, we consider two profiles that are widely used in the testing of numerical methods for equation (1): a Gaussian distribution and a rectangular box function. The first initial condition is a three-dimensional Gaussian distribution given by

$$u_0(x, y, z) = \exp\left(-\frac{(x-x_c)^2 + (y-y_c)^2 + (z-z_c)^2}{2\sigma^2}\right), \tag{10}$$

where the center is $(x_c, y_c, z_c) = (0, -0.25, 0.25)$ and the spread factor is $\sigma = 0.0414$. This distribution is characterized by the presence of small regions where the gradient changes rapidly, thus producing a challenge to the numerical simulation. The exact solution of a homogeneous equation (1) is given by

$$u(x, y, z, t) = \frac{2\sqrt{2}\sigma^3}{(2\sigma^2 + 4Dt)^{3/2}} \times \exp\left(-\frac{(\bar{x}-x_c)^2 + (\bar{y}-y_c)^2 + (\bar{z}-z_c)^2}{2\sigma^2 + 4Dt}\right), \tag{11}$$

where $(\bar{x}, \bar{y}, \bar{z}) = (x\cos(4t) + y\sin(4t), -x\sin(4t) + y\cos(4t), z - t)$. To test the ELLAM method for problems with discontinuous initial data, we select the second initial configuration to be the three dimensional box function

$$u_0(x, y, z) = \begin{cases} 1, & (x, y, z) \in [-0.05, 0.05] \times [-0.3, -0.2] \times [0.2, 0.3], \\ 0, & \text{otherwise.} \end{cases} \tag{12}$$

The corresponding exact solution of a homogeneous equation (1) is given by

$$u(x, y, z, t) = \frac{1}{8}\left(\operatorname{erf}\left(\frac{\bar{x}+0.05}{\sqrt{4Dt}}\right) - \operatorname{erf}\left(\frac{\bar{x}-0.05}{\sqrt{4Dt}}\right)\right) \times \left(\operatorname{erf}\left(\frac{\bar{y}+0.3}{\sqrt{4Dt}}\right) - \operatorname{erf}\left(\frac{\bar{y}+0.2}{\sqrt{4Dt}}\right)\right)\left(\operatorname{erf}\left(\frac{\bar{z}-0.2}{\sqrt{4Dt}}\right) - \operatorname{erf}\left(\frac{\bar{z}-0.3}{\sqrt{4Dt}}\right)\right), \tag{13}$$

where $\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-s^2)\, ds$ denotes the standard error function.

As a representative model run, we carry the simulation using a grid of size $\Delta h := \Delta x = \Delta y = \Delta z = 1/50$ and a time step of $\Delta t = \pi/20$. Figure 2 contains isosurfaces of the analytic and the ELLAM solutions at each of the ten steps of the simulation. The ELLAM solution at the final time $t = \pi/2$ for the initial Gaussian has an absolute error of magnitude 3.95839×10^{-4} in the L_2 norm and 2.71354×10^{-5} in the L_1 norm, while that of the initial box function has an L_2 norm of 1.30885×10^{-3} and an L_1 norm of 7.48053×10^{-5}. We observe that the ELLAM solution for either initial condition is very accurate and captures the details and the sharp fronts of the exact solution without suffering from any numerical artifacts. This accuracy is achieved using a relatively large time step which amounts to a large Courant number of about 15.7. With a further refinement of the grid, we observed even more accurate solutions.

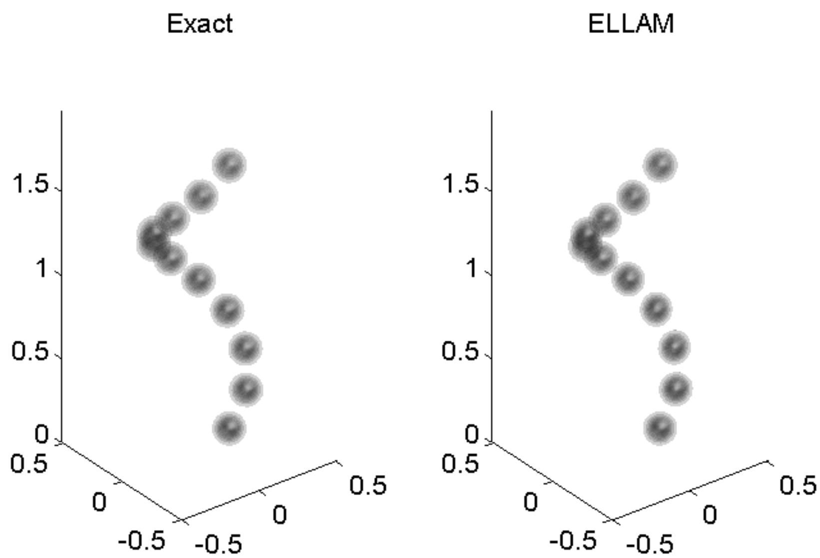
4.2. Diffusion in a Shear Flow

An interesting problem presented in [4] is the transport under the influence of a shear flow. Here we consider a three-dimensional version of this problem. The model equation (1) is solved using a velocity field of $\mathbf{v} = \langle 1 + 2y, 0, 0\rangle$ and a diffusion tesnor of $\mathbf{D} = 0.0001\mathbf{I}_3$ over a spatial domain of $[0, 1.4] \times [-0.05, 0.05]^2$. The analytic solution subject to a point source of mass M initial condition of the form $M\delta(x_0, 0)$ (where δ representes the Dirac delta function) is given by

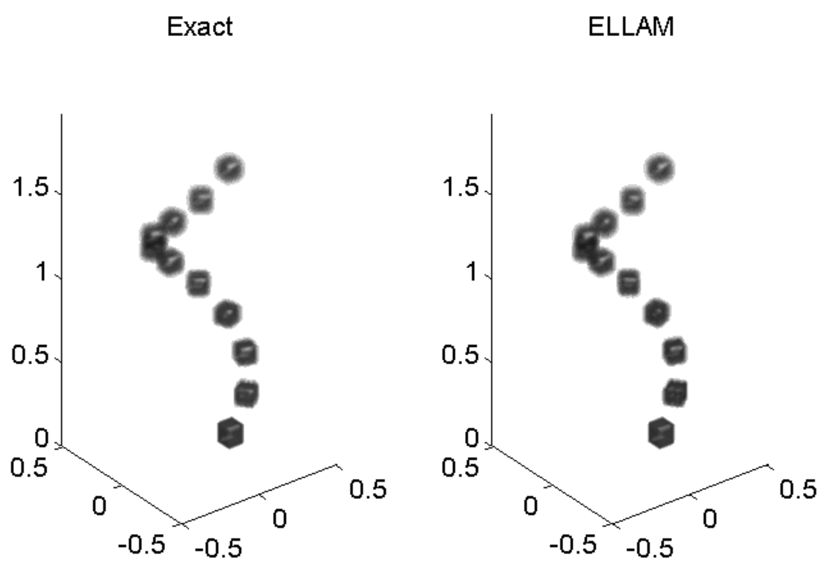
$$u(x,y,z,t) = \frac{M}{0.0004\pi t\sqrt{1+\frac{4t^2}{12}}} \times \exp\left(-\frac{(x-x_0-t-yt)^2}{0.0004t(1+\frac{4t^2}{12})} - \frac{y^2}{0.0004t} - \frac{z^2}{0.0004t}\right), \quad (14)$$

where we use the value $M = 0.002$. The source and sink term, computed accordingly, is $u(x, y, z, t)/(2t)$.

In the model problem we work with a finite initial condition at $t = 0.2$ and simulate over the time interval $[0.2, 1.2]$. As a representative model run, we simulate the problem with a discretization of the space-time domain of size $\Delta h = 1/200$ and $\Delta t = 1/10$ and present isosurfaces of the ELLAM solution and the analytic solution at times 0.7 and 1.2 in Figure 3. The norms of the absolute error in the ELLAM approximation at $t = 1.2$ are an L_2 norm of 3.00433×10^{-4} and an L_1 norm of 5.27674×10^{-6}. We observe that the ELLAM method captures the fine details of the exact solution without showing any traces of oscillations or numerical diffusion. All of this accuracy is achieved



(a) The Gaussian distribution



(b) The box function

Figure 2: Isosurfaces of the initial solution and the exact and ELLAM solutions in problem 4.1 at the ten time-steps of the simulation with the time interval $[0, \pi/2]$ using $\Delta h = 1/50$ and $\Delta t = \pi/20$

using only ten steps for the time interval [0.2, 1.2] which amounts to a relatively large time step.

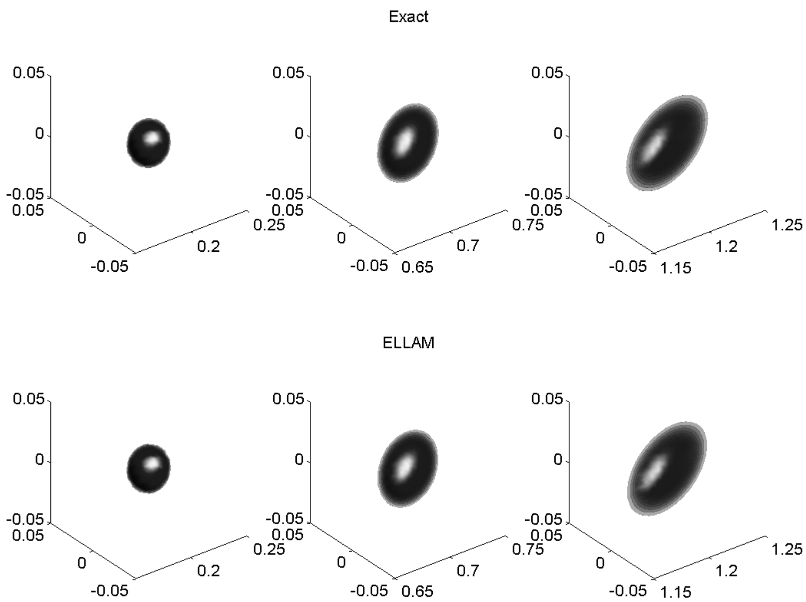


Figure 3: Isosurfaces of the initial condition, and the exact (top row) and ELLAM solutions (bottom row) at $t = 0.7$ and $t = 1.2$ for experiment 4.2 using $\Delta h = 1/200$ and $\Delta t = 1/10$

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