Mathematical Modelling and Analysis 2005. Pages 277–282
Proceedings of the 10^{th} International Conference MMA2005&CMAM2, Trakai
 ISBN 9986-05-924-0

ON ERROR ESTIMATES FOR ELLAM FOR CONVECTION-DIFFUSION EQUATIONS

H. WANG

Department of Mathematics, University of South Carolina

Columbia, South Carolina 29208, USA

E-mail: hwang@math.sc.edu

Abstract. We discuss the convergence analysis and error estimates for an Eulerian-Lagrangian method for transient convection-diffusion equations. An ε-uniform optimal-order error estimate is presented to show the strength of the scheme.
Key words: characteristic methods, transient convection-diffusion equations, error estimates, Eulerian-Lagrangian methods, singularly perturbed problem

1. Introduction

Transient convection-diffusion partial differential equations of the form

$$c_t + \nabla \cdot (\mathbf{v}(\mathbf{x},t)c) - \varepsilon \nabla^2 c(\mathbf{x},t) = f(\mathbf{x},t), \qquad (\mathbf{x},t) \in \Omega \times [0,T] \qquad (1.1)$$

arise in the mathematical model of petroleum reservoir simulation, environmental modeling, and other applications [4, 6]. Here $\mathbf{v}(\mathbf{x},t)$ is fluid velocity, $f(\mathbf{x},t)$ is a given function, and $c(\mathbf{x},t)$ is the concentration of a dissolved substance. $\Omega \subset \mathbb{R}^d$ is a bounded domain. $0 < \varepsilon << 1$ scales the diffusion and quantifies the convection-dominance of Eq. (1.1).

These problems admit solutions with moving steep fronts and complex structures, and present serious mathematical and numerical difficulties. Classical centered finite difference or finite element methods tend to generate numerical solutions with nonphysical oscillations. Upwinding techniques are widely used to stabilize the numerical approximations, but they often produce numerical solutions with excessive numerical diffusion that smears out the moving steep fronts and generates spurious grid orientation effects [4].

Characteristic methods have been developed to overcome the numerical difficulties by combining the convection term with the capacity term in the transient convection-diffusion equations, and carry out the temporal discretization via a characteristic tracking algorithm. Consequently, these methods reduce time truncation errors significantly and generate accurate numerical solutions even if large time steps and coarse spatial grids are used. However, many earlier characteristic methods often fail to conserve mass, which is of essential importance in applications.

The Eulerian-Lagrangian localized adjoint method (ELLAM) [2] was formulated to conserve mass and to treat general boundary conditions, while retaining the numerical advantages of earlier characteristic methods. The ELLAM is competitive with many numerical methods [9, 10] and has been used in applications [12]. In this paper we address the issues of error estimates for the ELLAM schemes for transient convection-diffusion equations.

2. The Eulerian-Lagrangian Localized Adjoint Method

Let $0 = t_0 < t_1 < \cdots < t_n < \cdots < t_N = T$ be a temporal partition of $[0, T]$ with $\Delta t_n = t_n - t_{n-1}$. In the ELLAM formulation the test functions $w(\mathbf{x}, t)$ are chosen from the Sobolev space $H^1(\Omega)$ for each time $t \in (t_{n-1}, t_n]$. The test functions $w(\mathbf{x}, t)$ are continuous in time except at time t_{n-1}, at which $w(\mathbf{x}, t)$ is left continuous and has right limit with respect to time t. Multiply Eq. (1.1) by such $w(\mathbf{x}, t)$, integrating the resulting equation on $\Omega \times (t_{n-1}, t_n]$, and incorporating the boundary condition (we assume noflow boundary for the sake of exposition of the ideas) yields a space-time weak formulation

$$\begin{aligned}
&\int_\Omega c(\mathbf{x}, t_n) w(\mathbf{x}, t_n)\, d\mathbf{x} + \int_{t_{n-1}}^{t_n} \int_\Omega \varepsilon \nabla w(\mathbf{y}, \theta) \cdot \nabla c(\mathbf{y}, \theta)\, d\mathbf{y} d\theta \\
&\quad - \int_{t_{n-1}}^{t_n} \int_\Omega c(\mathbf{y}, \theta) \Big[w_\theta(\mathbf{y}, \theta) + \mathbf{v}(\mathbf{y}, \theta) \cdot \nabla w(\mathbf{y}, \theta) \Big]\, d\mathbf{y} d\theta \qquad (2.1)\\
&= \int_\Omega c(\mathbf{x}, t_{n-1}) w(\mathbf{x}, t_{n-1}^+)\, d\mathbf{x} + \int_{t_{n-1}}^{t_n} \int_\Omega f(\mathbf{y}, \theta) w(\mathbf{y}, \theta)\, d\mathbf{y} d\theta,
\end{aligned}$$

where $w(\mathbf{x}, t_{n-1}^+) = \lim_{t \to t_{n-1}^+} w(\mathbf{x}, t)$ takes into account for the fact that $w(\mathbf{x}, t)$ might be discontinuous at time t_{n-1}.

In the ELLAM formulation [2, 10] the test functions $w(\mathbf{y}, \theta)$ are defined to satisfy the homogeneous hyperbolic equations, given by the hyperbolic part of the adjoint equations [10]

$$w_\theta(\mathbf{y}, \theta) + \mathbf{v} \cdot \nabla w(\mathbf{y}, \theta) = 0, \quad (\mathbf{y}, \theta) \in \Omega \times (t_{n-1}, t_n]. \qquad (2.2)$$

This equation can be rewritten as the following ordinary differential equation

$$\frac{dw(\mathbf{r}(\theta; \mathbf{x}, t_n), \theta)}{d\theta} = 0, \qquad w(\mathbf{r}(\theta; \mathbf{x}, t_n), \theta)\Big|_{\theta = t_n} = w(\mathbf{x}, t_n). \qquad (2.3)$$

along the characteristic curve $\mathbf{y} = \mathbf{r}(\theta; \mathbf{x}, t_n)$ which passes through $\mathbf{x}$ at time $\theta = t_n$. This equation shows that once they are defined in $\overline{\Omega}$ at time step t_n, the test functions $w(\mathbf{x}, t)$ are completely determined in the space-time domain $\overline{\Omega} \times (t_{n-1}, t_n]$ by a constant extension along the characteristic curves.

Applying a first-order Euler approximation along the characteristic curve to evaluate the source and sink term and the diffusion term yields

$$\begin{aligned}
&\int_{t_{n-1}}^{t_n}\int_{\Omega} f(\mathbf{y},\theta)\, w(\mathbf{y},\theta)\, d\mathbf{y}d\theta = \Delta t_n \int_{\Omega} f(\mathbf{x},t_n) w(\mathbf{x},t_n)\, d\mathbf{x} + E_f(c,w),\\
&\int_{t_{n-1}}^{t_n}\int_{\Omega} \varepsilon \nabla w(\mathbf{y},\theta)\cdot\nabla c(\mathbf{y},\theta)\, d\mathbf{y}d\theta \\
&\qquad = \Delta t_n \int_{\Omega} \varepsilon \nabla w(\mathbf{x},t_n)\cdot \nabla c(\mathbf{x},t_n)\, d\mathbf{x} + E_\varepsilon(c,w).
\end{aligned} \tag{2.4}$$

Here $E_f(c,w)$ and $E_\varepsilon(c,w)$ are the local truncation error terms due to the use of the Euler quadrature to the source and sink term and the diffusion term.

Incorporating Eq. (2.4) into the weak form (2.1), we obtain an Eulerian-Lagrangian reference equation for problem (1.1)

$$\begin{aligned}
&\int_{\Omega} c(\mathbf{x},t_n) w(\mathbf{x},t_n)\, d\mathbf{x} + \Delta t_n \int_{\Omega} \varepsilon\nabla w(\mathbf{x},t_n)\cdot\nabla c(\mathbf{x},t_n)\, d\mathbf{x}\\
&\quad = \int_{\Omega} c(\mathbf{x},t_{n-1}) w(\mathbf{x},t_{n-1}^+)\, d\mathbf{x} + \Delta t_n \int_{\Omega} f(\mathbf{x},t_n) w(\mathbf{x},t_n)\ d\mathbf{x}\\
&\qquad + E_f(c,w) - E_\varepsilon(c,w).
\end{aligned} \tag{2.5}$$

We point out that the ELLAM formulation (2.5) leads to a self-adjoint and coercive bilinear form for a non-self-adjoint transient convection-diffusion problem (1.1). Computationally, the discrete system is solved on a fixed Eulerian spatial grid at time step t_n even though (2.5) is an Eulerian-Lagrangian formulation. The characteristic tracking algorithm is carried out only to evaluate the first term on the right-hand side. Thus, this algorithm has no effect on the solution grid or the data structure of the discrete system at all. Therefore, the ELLAM formulation does not suffer from the complication of distorted grids which complicates many forward characteristic methods. Moreover, the ELLAM formulation leads to mass-conservative numerical methods [2, 11]and generates accurate numerical solutions with minimal numerical artifacts even if large time steps and spatial grids are used [9, 10].

3. On Error Estimates of ELLAM Schemes

In this section we address the issues on error estimates for ELLAM schemes for transient convection-diffusion equations. Let $W_p^m(0,1)$ be the Sobolev spaces [3] that consist of functions whose derivatives up to order-m are p-th Lebesgue integrable in $(0,1)$. Let $L^p(0,1) = W_p^0(0,1)$ and $H^m(0,1) = W_2^m(0,1)$. For any Banach space X, we introduce Sobolev spaces involving time

$$W_p^m(0,T;X) := \Big\{ f(x,t) : \Big\| \frac{\partial^\alpha f}{\partial t^\alpha}(\cdot,t)\Big\|_X \in L^p(0,T),\ 0\le\alpha\le m,\ 1\le p\le\infty \Big\}$$

$$\|f\|_{W_p^m(0,T;X)} := \begin{cases} \Big(\displaystyle\sum_{\alpha=0}^{m} \int_0^T \Big\|\frac{\partial^\alpha f}{\partial t^\alpha}(\cdot,t)\Big\|_X^p dt\Big)^{1/p}, \ 1\le p<\infty,\\ \displaystyle\max_{0\le\alpha\le m}\ \operatorname*{ess\ sup}_{(0,T)} \Big\|\frac{\partial^\alpha f}{\partial t^\alpha}(\cdot,t)\Big\|_X,\ \ p=\infty. \end{cases}$$

We also use the discrete norm $\|f\|_{\hat{L}^2(0,1)}$ in which the middle-point rule is used to evaluate the integral at each spatial cell. Similarly, in the discrete norm $\|f\|_{\hat{L}^p(0,T;X)}$ the temporal integral is replaced by a discrete summation sampled at the discrete time steps t_n for $n = 0, 1, \ldots, N$.

3.1. Optimal-order error estimates

The theoretical analysis for ELLAM schemes introduces further difficulties to the already complicated analyses of characteristic methods. These issues include simultaneous a priori estimates for unknowns in interior and at outflow boundaries, and those due to the special treatment of the boundary for the sake of mass conservation. The author and collaborators proved a generalized weighted Sobolev inequality, and utilized the inequality to derive an optimal-order error L^2 estimate

$$\begin{aligned}\|c_h - c\|_{\hat{L}^\infty(0,T;L^2(0,1))} \le K\Delta t\Big(&\|c_\tau\|_{L^2(0,T;W^{1,\infty}(0,1))} + \|c\|_{L^\infty(0,T;H^2(0,1))} \\ &+ \|f_\tau\|_{L^2(0,T;L^2(0,1))}\Big) + K(\Delta x)^2\|c_t\|_{L^2(0,T;H^2(0,1))} \qquad (3.1)\end{aligned}$$

and a superconvergence estimate

$$\begin{aligned}\|(c_h - c)_x\|_{\hat{L}^\infty(0,T;\hat{L}^2(0,1)} \le K\Delta t\Big(&\|c_\tau\|_{L^2(0,T;W^{1,\infty}(0,1))} + \|c\|_{L^\infty(0,T;H^3(0,1))} \\ &+ \|f_\tau\|_{L^2(0,T;L^2(0,1))}\Big) + K(\Delta x)^2\|c_t\|_{L^2(0,T;H^2(0,1))} \qquad (3.2)\end{aligned}$$

for the ELLAM scheme with piecewise-linear finite-element approximations for the one-dimensional analogue of problem (1.1) in $\Omega = (0,1)$ [11]. Here c_τ refers to the material derivative of c along the characteristic curves. K is a constant that is independent of the mesh parameters Δt and Δx, but could potentially depend on ε. We notice that the coefficients of Δt are much smaller than the coefficients of Δx. So this estimate theoretically justifies the use of large time steps in ELLAM schemes.

However, these analyses were based on a generalized weighted Sobolev inequality the authors proved, which in turn depends on the Sobolev embedding theorem $H^1(\Omega) \hookrightarrow C(\overline{\Omega})$. This is true only in one space dimension. Hence, the analyses would not carry over to multi-dimensional problems. An alternative approach was developed to derive an optimal-order L^2 error estimate and a superconvergence estimate for the ELLAM scheme for problem (1.1) in multiple space dimensions in [8]. A different but related method to the ELLAM is the characteristic mixed finite element method [1], which uses piecewise-constant space-time test functions. As with the standard mixed finite element method, a coupled system results for both the concentration and the diffusive flux. The theoretically proven error estimate is $O((\Delta x)^{\frac{3}{2}})$ for grid size Δx, which is suboptimal by a factor $O((\Delta x)^{\frac{1}{2}})$.

3.2. An ε-uniform optimal-order error estimate

In the estimate (3.1), the coefficients K and the norms of the true solution c depend on ε. Namely, as ε decreases, the coefficients could potentially increase. This type of error estimates, which has also been proved for many other numerical methods for convection-diffusion equations, has drawn some debates. Some researchers argue that it is useless in practice since the coefficients could potentially blow up as ε tends to zero. They advocate an estimate that holds uniformly with respect to ε. Others argue that the size of diffusion is always fixed in practice. For smaller ε, the true solution c will have steeper fronts and hence requires refined spatial grids and time steps. In any case, both sides agree that an ε-uniform error estimate would be ideal.

In the context of stationary convection-diffusion equations, these issues have been addressed either by the use of upwinding techniques that stabilize the numerical methods or by adoption of a delicately designed local grid refinement near the boundary layer that was originally due to Shishkin ([5, 7] and the references therein). In particular, the Shishkin mesh approach has successfully resolved the boundary layer problem with a simple piecewise-uniform grid. More importantly, an ε-uniform L^∞ error estimate has been proved for numerical methods with Shishkin mesh.

In the context of transient convection-diffusion equations the situation becomes less obvious, because the dynamic steep fronts do not always coincide with computational mesh in general due to the complex structures (especially in multiple space dimensions). This is somewhat similar to the reason why L^∞ error estimate is not very suited for the numerical methods for hyperbolic conservation laws. In this conference the author has presented his work on an ε-uniform error estimate for the ELLAM scheme with a uniform space-time partition (and with no upwinding or stabilization introduced in the scheme) for problem (1.1) in one space dimension

$$
\begin{aligned}
&\|c_h - c\|_{\hat{L}^\infty(0,T;L^2)} + \sqrt{\varepsilon}\|(c_h - c)_x\|_{\hat{L}^2(0,T;L^2(0,1))} \\
&\quad \le K\Delta t(\sqrt{\varepsilon}\|c_o\|_{H^2} + \|c_o\|_{H^1} + \|f_\tau\|_{L^2(0,T;L^2(0,1))} \\
&\qquad + \|f\|_{L^2(0,T;H^1(0,1))}) + K(\min\{h, \Delta t\} + h^2)\|c_o\|_{H^2(0,1)} \\
&\qquad + K\lambda h^2(\|c_o\|_{H^3(0,1)} + \|f\|_{L^2(0,T;H^3(0,1))}).
\end{aligned} \tag{3.3}
$$

Here the constant K is independent of the true solution c and the parameter ε. The parameter $\lambda = 0$ if the Courant number is less than one and 1 otherwise. c_0 is the prescribed initial condition for c. The derivation of this error estimate is very long and technical, and hence will be submitted elsewhere.

We note that the coefficients in the estimate (3.3) are independent of ε or any norm of the true solution c, but depend only on the initial and right-hand side data c_0 and f. Using the theory of interpolation of Sobolev spaces or Besov spaces and the L^2-stability estimates of problem (1.1) and the ELLAM scheme, we also derive an ε-uniform estimate for the ELLAM scheme when the given data has less or minimal regularity. Finally, it is easy to check that for the true solution with an exponential layer, the weighted norm on the left-hand side of (3.3) is comparable to L^∞ norm. Hence, the estimate (3.3) is optimal since an ε-uniform L^∞ estimate is generally impossible for numerical methods to transient convection-diffusion equations. In summary, the estimate (3.3) justifies the strength of the ELLAM scheme theoretically.

References

[1] T. Arbogast and M.F. Wheeler. A characteristic-mixed finite element method for advection-dominated transport problems. *SIAM J. Numer. Anal.*, 404 – 424, 1995.

[2] M.A. Celia, I. Herrera T.F. Russell and R.E. Ewing. An Eulerian-Lagrangian localized adjoint method for the advection-diffusion equation. *Advances in Water Resources*, **13**, 187 – 206.

[3] L.C. Evans. Partial Differential Equations. Technical Report 19, American Mathematical Society, Rhode Island, 1998.

[4] R.E. Ewing (Ed.). The Mathematics of Reservoir simulation. Research Frontiers in Applied Mathematics. *SIAM, Philadelphia*, **1**, 1984.

[5] P.A. Farrell, A.F. Hegarty, and E. O'Riordan J.J.H. Miller and G.I. Shishkin. *Robust Computational Techniques for Boundary Layers. Applied Mathematics*, volume 16. Chapman & Hall/CRC.

[6] R. Helmig. *Multiphase Flow and Transport Processes in the Subsurface.* Springer Verlag, Berlin, 1997.

[7] H.-G. Roos, M. Stynes and L. Tobiska. *Numerical Methods for Singularly Perturbed Differential Equations.* Springer-Verlag, Berlin, 1996.

[8] H. Wang. An optimal-order error estimate for an ELLAM scheme for two-dimensional linear advection-diffusion equations. *SIAM J. Numer. Anal.*, **37**, 1338 – 1368, 2000.

[9] H. Wang, H.K. Dahle, R.E. Ewing, M.S. Espedal, R.C. Sharpley and S. Man. An ELLAM scheme for advection-diffusion equations in two dimensions. *SIAM J. Sci. Comput.*, 2160 – 2194, 1999.

[10] H. Wang, R.E. Ewing, and M. Al-Lawatia G. Qin, and S.L. Lyons and S. Man. A family of Eulerian-Lagrangian localized adjoint methods for multi-dimensional advection-reaction equations. *J. Comput. Phys.*, **152**, 120 – 163, 1999.

[11] H. Wang, R.E. Ewing and T.F. Russell. Eulerian-Lagrangian localized methods for convection-diffusion equations and their convergence analysis. *IMA J. Numer. Anal.*, **15**, 405 – 459, 1995.

[12] H. Wang, D. Liang, and S.L. Lyons R.E. Ewing and G. Qin. An approximation to miscible fluid flows in porous media with point sources and sinks by an Eulerian-Lagrangian localized adjoint method and mixed finite element methods. *SIAM J. Sci. Comput.*, **22**, 561 –581, 2000.