On the role of tracking on Eulerian–Lagrangian solutions of the transport equation

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We investigate the effect of tracking errors on the accuracy and stability of Eulerian–Lagrangian methods (ELMs) for the solution of the transport equation. A combination of formal analysis and numerical experimentation demonstrates that the effect is severe. Even moderate tracking errors substantially affect the preservation of the zeroth, first and second moments of concentration (mass, phase and diffusion) and may lead to the instability of otherwise stable and very accurate ELMs. The use of accurate tracking algorithms is strongly recommended for Eulerian–Lagrangian simulations involving complex flows. © 1998 Elsevier Science Limited. All rights reserved

Key words: transport equation, Eulerian–Lagrangian methods, tracking methods, mass conservation, numerical experimentation, accuracy analysis, stability analysis.

1 INTRODUCTION

Many numerical methods have been proposed to solve the advection–diffusion equation.1 Among the several classes of proposed techniques, Eulerian–Lagrangian methods (ELMs) are generally recognized as very attractive when advection is dominant.2–10 The attractive numerical properties of ELMs stem from the adoption of customized techniques for each transport process: typically, advection is solved by the backward method of characteristics, while diffusion is solved by centered finite elements or finite differences. This decoupling strategy eliminates Courant number restrictions associated with Eulerian methods6 and provides an efficient way to handle processes with very different time scales.11

In spite of their attractive numerical properties and their increasing popularity in surface12–16,11 and subsurface17–20 water applications, the use of ELMs is hindered by the fact that they do not inherently conserve mass, either locally or globally.21,2,3,18,22–24 Mass errors result primarily from: (1) inaccurate tracking of the characteristic lines; (2) the use of nonconservative flow fields; (3) errors in the evaluation of conditions at the feet of the characteristic lines; and (4) approximations in the treatment of boundary conditions. Indeed:

(a) Both inaccurate tracking of characteristic lines and nonconservative flow fields (e.g. flow fields where the continuity equation is not exactly verified due to numerical errors) lead to the incorrect positioning of the feet of characteristic lines [Fig. 1(a and b)]. On an elemental basis, the consequence is an improper definition of the region where integrals are evaluated at time \( n \) (\( n + 1 \) being the current time step).18 Local mass errors are thus generated and there is no mechanism to compensate for them globally.

(b) The effect of nonconservative flows is aggravated when, as it is the case for most ELM models, the non-conservative transport equation is used. In order to treat the advective term in its Lagrangian form, these models write the transport equation as:

\[
\frac{\partial c}{\partial t} + \nabla \cdot (u \nabla c) = \nabla \cdot (D \nabla c) - \frac{\partial u}{\partial x_i} \frac{\partial c}{\partial x_i}, \quad i = 1, 2, 3, \tag{1}
\]

where \( c \) is the concentration; \( u_i \) are the components of velocity in each spatial dimension \( x_i \); \( D_{ij} \) is the diffusion coefficient tensor and \( t \) is time. Furthermore, the models assume that flow continuity is inherently respected, i.e.:

\[
\frac{\partial u_i}{\partial x_i} = 0, \tag{2}
\]
and drop the ‘source’ term that contains the divergence of the flow.

(c) Errors in the evaluation of concentrations at the feet of the characteristic lines can generate local mass errors, both when interpolation\(^2\) [such as the linear interpolator ELM, as illustrated in Fig. 1(c)] or quadrature methods\(^2\)\(^2\) are used. For the transport equation with uniform coefficients and a uniform grid, formal analysis of ‘interpolation ELMs’ shows that these local mass errors do not translate into significant global mass errors, unless significant aliasing occurs at high frequencies.\(^2\). For ‘quadrature ELMs’ a careful choice of the numerical integration rule is necessary to avoid mass imbalances.\(^2\)

(d) Incorrect implementation of boundary conditions can lead to significant mass imbalances.\(^3\) To minimize this problem, Eulerian–Lagrangian localized adjoint methods (ELLAMS)\(^1\)^\(^8\),\(^1\)^\(^9\),\(^2\)^\(^4\) implement boundary conditions through the use of space–time weighting functions, leading to global mass conservation when other sources of mass imbalances are not present.

Although mass conservation in ELMs has been broadly recognized as a significant problem\(^2\),\(^3\),\(^1\)^\(^8\),\(^2\)^\(^2\)–\(^2\)^\(^4\) this work represents, to our knowledge, the first systematic investigation of the effect of inaccurate tracking on the numerical properties of ELMs. We show that tracking errors not only affect mass, but can also introduce significant phase errors and numerical diffusion. Moreover, we show that inaccurate tracking can lead to instability of otherwise stable ELMs.

The paper is divided into five sections beyond this introduction. The significance of the tracking errors and resulting mass imbalances in real estuarine systems is illustrated in Section 2, through two-dimensional transport simulations for the Tejo estuary, Portugal. This provides the motivation and context for the remaining sections, which abstract the problem into a simple one-dimensional framework. Section 3 describes the formulation of a reference ELM, including a mechanism to introduce tracking errors. Section 4 uses truncation error analysis to examine the errors introduced or magnified by inexact tracking. The influence of dimensionless parameters on selected numerical properties of solutions with tracking errors is then examined through numerical experimentation (Section 5). Finally, Section 6 summarizes the results and discusses their implications.

2 CONTEXT

We examine, in this section, the tracking errors in a complex estuarine system and their impact on the transport of a conservative tracer plume. The Tejo estuary [Fig. 2(a)] and the two-dimensional flow and transport models TEA–NL\(^2\)^\(^5\),\(^2\)^\(^6\) and ELA\(^1\)^\(^8\) are used as reference. The formulation of the two models is briefly reviewed in Appendix A.

The Tejo estuary, located in Portugal, is forced by ocean tides and by regulated river discharges. In combination with a complex geometry and bathymetry, these forcings lead to complicated circulation and flushing patterns [Fig. 2(b)]. For simplicity, tidal flats were artificially ‘deepened’ in our simulations [Fig. 2(a)] and play no role in the conservation errors described herein.

Flow was simulated with the model TEA–NL only for the dominant tidal constituent ($M_2$) and its major harmonics ($M_4$, $M_6$, $M_8$ and $Z_0$). With the exception of advection, all nonlinear processes were included. Mass conservation is respected only approximately, both locally and globally [Table 1, Fig. 3(a and b)] since TEA–NL approximates the continuity equation by finite elements. Maximum global errors are of the order of 2.5 $\times$ 10\(^{-4}\)%/s (scaled by the volume of the estuary at rest), while maximum elemental errors are of the order of 0.5%/s (scaled by the elemental volume).

Considerable mass errors occur both at land and ocean boundaries. The treatment of elevation as an essential boundary condition, by dropping the continuity equation and evaluating the velocity using the momentum equations, introduces considerable mass errors at open boundaries,\(^2\)^\(^7\) while the treatment of normal flow as a natural boundary condition allows mass imbalances through land boundaries.

![Fig. 1. Sources of mass errors in ELMs: (a) back-tracking of the characteristic lines, with tracking errors in one characteristic line only, for a Courant number of 1; (b) use of non-conservative flow field; and (c) interpolation at the feet of the characteristic lines.](image-url)
The generation of mass errors inside the domain is not fully understood yet, but studies conducted for wave continuity equation models suggest that local mass errors are associated with regions of large bathymetric gradients and rapidly changing geometry.28

ELA12 is one of the first Eulerian–Lagrangian transport models developed for coasts and estuaries. For this application, ELA was modified to allow for alternative tracking strategies. From the many different techniques21,12,3,14,29,15,30–32 that have been considered to perform tracking in transport models, we selected three (Appendix B, Table 2):

- one-step backward Euler (BE), where the tracking and diffusion time steps coincide;
- multi-step backward Euler (MSE), where the tracking time step is a submultiple of the diffusion time step;
- fifth-order Runge–Kutta (RK), where the time step is dynamically adjusted to meet a user-specified spatial accuracy criterion. This method is constructed from the fourth-order Runge–Kutta displayed in Table 2, as discussed in Appendix B.

These schemes are representative of low- and high-order integration rules rather than being intended as optimal accuracy choices. The one-step Euler method14 is now rarely used, while both the multi-step Euler33 and the fifth-order Runge–Kutta methods11 are often used in current practice.

Tracking errors, estimated by closure errors as described in Appendix C, were computed for five particles released at locations with different flow characteristics [Fig. 2(a)], using various time steps and lengths of simulation (Table 3). Choices of the tracking time steps are loosely representative of those made in published applications.33,14,30–32

The results (Table 4) show that while tracking errors can be made quite small (e.g. RK simulations), they are often significant to very large (e.g. BE and most MSE
simulations). Efficiency considerations aside, tracking errors depend primarily on the strategy adopted for the tracking subtime step and on flow character. When the time step is locally adjusted to control tracking errors, then dependence on flow is reduced or eliminated.

In particular, we note that:
- RK tracking with adjustable time step is very accurate regardless of the initial location and pathway of the particle;
- Euler methods lead to tracking errors whose magnitude is strongly accentuated by sharp velocity gradients and which can be very large even for tracking time steps as small as 1 min;
- reducing the tracking subtime step in MSE tracking considerably improves accuracy, but errors in certain regions of the domain remain quite significant even for $\Delta t = 10/10$.

Transport simulations using ELA with RK and MSE tracking were conducted for three tidal cycles with two alternative diffusion time steps ($\Delta t = 10$ min and 1 h). The transport problem consists of an instantaneous plume being released during flood at the downstream end of the entrance channel [Fig. 2(c)]. Mass errors (Table 1) are shown in Fig. 4.

Although RK tracking is very accurate, with negligible closure errors, the associated transport simulation still has mass errors of up to 20% [Fig. 4(a)]. These transport mass errors are due to a combination of all other effects discussed.
in Section 1. This includes the inability of TEA–NL to preserve the divergence-free characteristics of the flow (Fig. 3); ELA, which uses a nonconservative form of the transport equation, cannot compensate for this effect.

The tracking part of the transport mass errors, for simulations using MSE methods, can be roughly separated from the total by subtracting the transport mass errors for the corresponding (presumably tracking error-free) RK simulation. This approach suggests, for example, that MSE tracking increases total transport mass errors by 20% for $\Delta t = 10$ min and up to 100% for $\Delta t = 1$ h [Fig. 4(b)].

The above analysis illustrates the potential for mass imbalances that results from poor tracking. Because this potential is large, there is a clear motivation to search for a better understanding of the influence of the magnitude of the tracking errors on mass conservation and other numerical properties of Eulerian–Lagrangian transport simulations. The following sections abstract the problem to a simple enough level that enables interpretation of cause–effect relationships. The above analysis also suggests that the use of locally nonconservative flow fields may be an equally important source of transport mass errors. This problem is beyond the scope of this investigation, but will be addressed in future research.

3 NUMERICAL FORMULATION

As a basis for a systematic analysis of the impact of tracking errors, we now consider the solution of the one-dimensional, simplified form of the transport equation:

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2},$$  

(3)

where $u$ and $D$ are both positive and constant. Assuming a uniform grid with linear elements, the weighted residual statement for a generic Eulerian–Lagrangian finite element method can be written as:

$$\int_\Omega \left\{ \int_\Omega f_k c n + 1 - c_i \right\} \frac{\partial c}{\partial x} d\Omega + \Psi = 0,$$

(4)

where we integrated by parts the diffusion residual and omitted the explicit representation of the resulting boundary terms, $\Psi$. Linear shape and weighting functions, $f_k$, are assumed for simplicity. The superscript $n + 1$ represents the time level at which concentrations are being evaluated and $x$ denotes quantities calculated at the feet of the characteristic lines (at time level $n$). The time weighting factor, $\alpha$, was set to 0.5 in all simulations.

Concentrations at the feet of the characteristic lines ($c^e$) are obtained by linear interpolation:

$$c_i^e = \sum_{j=1}^2 \phi_j(\theta) c_i^{n+1} = c_i^n - \frac{1}{2} (c_{i-1}^n - c_{i+1}^n).$$

(5)

Table 3. Definition of particle runs

<table>
<thead>
<tr>
<th>Run</th>
<th>Time step (minutes)</th>
<th>Simulation length (tidal cycles)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1, 5, 15, 30, 60</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td>2, 2.25, 2.5, 2.75, 3</td>
</tr>
</tbody>
</table>

1Linear interpolation at the feet of the characteristic lines was selected because it is the simplest method to achieve our purposes. The reader should keep in mind, though, that this method is known to lead to substantial numerical diffusion, and is not a frequent choice in practice (e.g. see discussion in Ref. 7).
Table 4. Maximum and (minimum) closure errors

<table>
<thead>
<tr>
<th>Particle Time step analysis (Run 1)</th>
<th>Simulation Length analysis (Run 2)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Runge–Kutta</td>
</tr>
<tr>
<td>1 0.9 × 10⁻¹ (0.2 × 10⁻³)</td>
<td>9.57 (2.01)</td>
</tr>
<tr>
<td>2 0.2 × 10⁻¹ (0.7 × 10⁻³)</td>
<td>5.30 (1.16)</td>
</tr>
<tr>
<td>3 0.4 × 10⁻¹ (0.4 × 10⁻⁵)</td>
<td>5.47 (0.87)</td>
</tr>
<tr>
<td>4 0.2 × 10⁻⁵ (0.1 × 10⁻³)</td>
<td>0.63 (0.1 × 10⁻¹)</td>
</tr>
<tr>
<td>5 0.3 × 10⁻⁸ (0.8 × 10⁻¹⁵)</td>
<td>1 × 10⁻¹ (0.5 × 10⁻⁵)</td>
</tr>
</tbody>
</table>
on the role of tracking on the transport equation

\[ \frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = \text{D} \frac{\partial^2 c}{\partial x^2} + \frac{\partial}{\partial x}(\alpha \text{D} \frac{\partial c}{\partial x} + \text{Pe}) \]

Fig. 4. Mass errors for three tidal cycles for Euler and Runge–Kutta tracking with time steps of 10 and 60 min; (b) mass error differences between Euler and Runge–Kutta tracking techniques.

where \( \theta_i \in [0, 1] \) represents the computed position of the foot of characteristic line for node i within the receiving element, and \( \beta_i, \sigma_i \) and \( \psi_i \) are the effective Courant number, its integer part and its fractional part, respectively:

\[ \beta_i = \frac{u_{\Delta t}}{\Delta x}, \quad \Lambda_i = Cu - \Lambda_i \]

\[ \sigma_i = \text{int}(\beta_i) \]

\[ \delta_i = \beta_i - \sigma_i \]

where \( Cu \) is the Courant number and \( \Lambda_i \) is a node- and time-dependent tracking error. This tracking error is introduced in the formulation to enable, in later sections, the systematic study of the importance of tracking inaccuracies on the transport simulation.

The finite difference analog of eqn (4) can be written as:

\[ \frac{1}{6} (A^{n+1} - A^1) = \alpha \text{D}^x B^{n+1} + (1 - \alpha) \text{D}^x B^1, \]

where \( \text{D}^x = CuPe \) and

\[ A^n = c_{i-1}^n + 4c_i^n + c_{i+1}^n \]

\[ B^n = c_{i-1}^n - 2c_i^n + c_{i+1}^n \]

\[ A^1 = [c_{i-1}^n - \epsilon_{i-1} + 4c_i^n - \epsilon_i + c_{i+1}^n - \epsilon_{i+1}] \]

\[ - \{ \partial_{i-1}[(c_i^n - \epsilon_i) - c_{i-2}^n - \epsilon_{i-1}] \}

\[ + 4\partial_i(c_i^n - \epsilon_i) - \epsilon_i \]

\[ + \partial_{i+1}[(c_{i+1}^n - \epsilon_{i+1}) - c_{i+2}^n - \epsilon_{i+2}] \}

\[ B^1 = [c_{i-1}^n - \epsilon_{i-1} + 2c_i^n - \epsilon_i + c_{i+1}^n - \epsilon_{i+1}] \]

\[ - \{ \partial_{i-1}[(c_i^n - \epsilon_i) - c_{i-2}^n - \epsilon_{i-1}] \}

\[ - 2\partial_i(c_i^n - \epsilon_i) + \epsilon_i \]

\[ + \partial_{i+1}[(c_{i+1}^n - \epsilon_{i+1}) - c_{i+2}^n - \epsilon_{i+2}] \}

\[ \text{where} \quad \theta = -\frac{\Delta t}{6} + \frac{4\Lambda_i + \Lambda_{i+1}}{6} \]

\[ (1 - \alpha) \text{D}^x (\Lambda_i - 2\Lambda_i + \Lambda_{i+1}) \frac{\Delta x}{\Delta t} \]

\[ \psi = \left( \frac{Cu^2}{2} - Cu \right) \int \text{Cu} \]

\[ + \psi_2 \left( \frac{(\int Cu)^2}{2} + \psi_1 \right) \frac{\Delta x^2}{\Delta t} \]

and

\[ \psi_1 = \frac{1}{\int Cu} \left( \frac{\sigma_i + 4\sigma_i + \sigma_{i+1}}{6} \right) \]

\[ + (1 - \alpha) \text{D}^x (\sigma_i - 2\sigma_i + \sigma_{i+1}) \]

\[ \psi_2 = \frac{2}{(\int Cu)^2} \left( \frac{\sigma_i^2 + 4\sigma_i^2 + \sigma_{i+1}^2}{12} \right) \]

\[ + (1 - \alpha) \text{D}^x \left( \frac{\sigma_i^2 - 2\sigma_i^2 + \sigma_{i+1}^2}{2} \right) \]

\[ \psi_3 = \left( \frac{1}{6} + (1 - \alpha) \text{D}^x \right) \left( \frac{\sigma_i + 3}{2} \right) \Lambda_i \]

\[ + \left( \frac{4}{6} - 2(1 - \alpha) \text{D}^x \right) \left( \frac{\sigma_i + 1}{2} \right) \Lambda_i \]

\[ + \left( \frac{1}{6} + (1 - \alpha) \text{D}^x \right) \left( \sigma_{i+1} - \frac{1}{2} \right) \Lambda_{i+1} \]

Two particular cases are worth considering:
In the presence of tracking errors, different nodes will, in general, have different truncation errors. Differences in nodal errors will generate energy in frequencies that cannot be resolved by the grid. The energy associated with these Fourier components is then folded to the zero-frequency, generating mass errors. The mechanism that creates mass errors can be examined by considering a simple case, in which only one characteristic line has a tracking error [Fig. 1(a)]. The concentration field (and the local mass) is exact in all elements except those containing the foot of the characteristic line with the tracking error. Since mass errors in the affected elements cannot compensate each other, the total mass will not be preserved.

5 NUMERICAL EXPERIMENTATION

5.1 Experimental design

Numerical experimentation provides further insight into the influence of tracking errors on the concentration field. We considered the classical problem of a one-dimensional Gauss hill transported by a uniform steady flow. Tracking errors, characterized by a normal distribution with zero mean and varying standard deviation, were applied at each node at each time step. The dependence of resulting errors on selected dimensionless parameters was then analyzed using the error measures of Table 5. The numerical experiments are organized in three tests (Table 6), each examining the influence of a dimensionless parameter: magnitude of the tracking errors ($\epsilon$/$\Delta x$), Péclet number ($Pe$) and dimensionless standard deviation of the Gauss hill ($\sigma$/$\Delta x$), representing the steepness of the concentration gradients.

To study the impact of the magnitude of the tracking errors (test 1), we selected standard deviations between 0 and 100%, well within the range suggested by our two-dimensional analysis for the Tejo estuary (Section 2), where tracking errors even reached 1000% (see Table 4, for the one-step Euler tracking). For the study of the effect of the steepness of the concentration gradients (test 2), several standard deviations of the Gauss hill were selected, ranging from poor ($\sigma$/$\Delta x = 1$) to excellent plume discretization ($\sigma$/$\Delta x = 20$). Test 3 assesses the importance of diffusion by covering a wide spectrum of diffusion coefficients, ranging from advection-dominated ($Pe = \infty$) to diffusion-dominated transport ($Pe = 0.5$).

All runs were generated with the reference method presented in Section 3, for $Cu = 1$. In the absence of tracking errors, the solution of advection is exact, thus minimizing (but not eliminating since the effective Courant number, $\beta e$, will not be kept at 1) the noise introduced by other sources of errors in ELMs (e.g. interpolation or quadrature errors). A long enough domain was used to prevent boundaries from interfering with the simulation (2301 nodes with a constant grid spacing of 100 m).

Several ‘seeds’ (initial value used in the generation of the random tracking errors) were considered, in order to provide different distributions of tracking errors, for each standard deviation. The simulations were run for a period large enough (2000 time steps) to provide series of random numbers representative of the chosen statistical distribution.

\begin{equation}
\Gamma = \frac{1}{2} ( f^2 - \Phi ) \frac{\partial^2 \psi}{\partial x^2},
\end{equation}

where $\Phi$ is the fractional part of the Courant number. Eqn (12) establishes the dependence of the truncation error solely on the fractional part of the Courant number. For uniform tracking errors ($\Delta t = \Delta x, \beta_i = \beta$ and $\sigma = \sigma_i$), eqns (10) and (11) reduce to:

\begin{equation}
\Gamma = -\Lambda \Delta x \frac{\partial c}{\partial x} + \frac{1}{2} \frac{\partial^2 ( f^2 - \Phi )}{\partial x^2} \frac{\partial^2 \psi}{\partial x^2} + \sigma - \chi \frac{\Phi^2}{2} \frac{\partial^2 \psi}{\partial x^2} \frac{\partial^2 \psi}{\partial x^2} + \left( \sigma + \frac{1}{2} \Lambda \right) \frac{\Delta x^2 \frac{\partial^2 \psi}{\partial x^2}}{\Delta t \frac{\partial^2 \psi}{\partial x^2}} \frac{\partial^2 \psi}{\partial x^2},
\end{equation}

where $\chi$ is the integer part of the Courant number.

A comparison of the above equations shows that tracking errors reduce the order of convergence of the method, introduce phase errors and create an additional source of numerical diffusion. In particular:

- Convergence becomes $O(\Delta x)$ rather than $O(\Delta x^2)$.
- Phase errors, which did not occur in the absence of tracking errors, are now a function of the magnitude and distribution of tracking errors and of the diffusion coefficient.
- Tracking errors create the potential for instability since the added numerical diffusion can be positive or negative, depending on the specific tracking errors. This problem may be critical when inherently less-diffusive ELMs are used (for instance, integration ELMs).
- Truncation errors are strongly affected not only by the magnitude of the tracking errors, but also by their spatial variability. In particular, errors in the first and second moments depend on the diffusion coefficient only when tracking errors vary in space.
- Uniform tracking errors reduce phase errors to a ‘rigid-body’ shift, but do not eliminate the potential for instability since the added numerical diffusion can still be negative.
5.2 Results and discussion

The results are shown in Figs 5–14, and consist primarily on time series of error measures and associated statistics.

5.2.1 Overall impact of tracking errors

Consistently with our formal analysis, numerical experimentation shows that inexact tracking introduces significant errors on the zeroth, first and second moments of concentration even in the presence of small tracking errors (Figs 5 and 6). In addition, tracking errors tend to induce a very distinctive ‘signature’ in the concentration field, characterized by abrupt concentration ‘bumps’ (Fig. 5) with no apparent spatial or temporal pattern. We interpret these ‘bumps’ as the result of the lack of coherence of the tracking errors in adjacent nodes.

\[
\mu_x(t) = 1 - \frac{\int_{x} x \left( \frac{\int_{\text{num}} c_{\text{num}} dx}{\int_{\text{max}} dx} \right)^2 c_{\text{ex}} dx}{\int_{x} x \left( \frac{\int_{\text{num}} c_{\text{num}} dx}{\int_{\text{max}} dx} \right)^2 c_{\text{num}} dx}
\]

Scaled numerical diffusion

\[
\mu' = \left\{ \begin{array}{ll}
\frac{\int_{x} x \left( \frac{\int_{\text{num}} c_{\text{num}} dx}{\int_{\text{max}} dx} \right)^2 c_{\text{ex}} dx}{\int_{x} x \left( \frac{\int_{\text{num}} c_{\text{num}} dx}{\int_{\text{max}} dx} \right)^2 c_{\text{num}} dx} & \text{with tracking errors} \\
\frac{\int_{x} x \left( \frac{\int_{\text{num}} c_{\text{num}} dx}{\int_{\text{max}} dx} \right)^2 c_{\text{ex}} dx}{\int_{x} x \left( \frac{\int_{\text{num}} c_{\text{num}} dx}{\int_{\text{max}} dx} \right)^2 c_{\text{num}} dx} & \text{without tracking errors}
\end{array} \right.
\]

Discrete $L_2$-normal

\[
L_2(t) = \frac{1}{\mu(t)} \left[ \sum_{i} \left( \frac{c_{\text{num}} - c_{\text{ex}}}{c_{\text{num}}} \right)^2 \right]^{1/2}
\]

<table>
<thead>
<tr>
<th>Test</th>
<th>$Cu$</th>
<th>$\lambda$ (%)</th>
<th>$\sigma$/$\Delta x$</th>
<th>$Pe$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0.1, 10, 25, 50, 75, 100</td>
<td>10</td>
<td>$\infty$</td>
</tr>
<tr>
<td>1A</td>
<td>0.5</td>
<td>0.1, 10, 25, 50, 75, 100</td>
<td>10</td>
<td>$\infty$</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>25</td>
<td>1, 3, 6, 10, 15, 20</td>
<td>$\infty$</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>25</td>
<td>10</td>
<td>$\infty$, 100, 25, 5, 2, 1, 0.5</td>
</tr>
</tbody>
</table>
of their dependence on controlling parameters such as the magnitude of tracking errors. In contrast, numerical diffusion clearly grows with larger tracking errors [Fig. 6(c)].

Since the effective Courant number will not be kept at 1 due to the tracking errors, it could be argued that the order of magnitude of the observed errors is due to the specific ELM selected. To analyze this hypothesis, we compare solutions with inexact tracking and a flow-induced Courant number of 1, and solutions without tracking errors but with a Courant number that leads to the maximum numerical diffusion ($Cu = 0.5$, dashed lines in Fig. 6). Mass and phase errors are both very small when tracking is exact [Fig. 6(a and b)]. Numerical diffusion, though, can be partially attributed to the selected ELM: the second moment of solutions with inexact tracking is of the same order of magnitude of the second moment in the absence of tracking errors [Fig. 6(c)].

The next sections discuss the dependence of each error measure—mass, phase and numerical diffusion—on dimensionless parameters.

5.2.2 Mass errors

Within a single simulation, the dependence of mass errors on the dimensionless numbers $e/\Delta x$, $e/\Delta t$ and $D^*$ is mostly inconclusive [dashed lines in Fig. 7(a to c)]. However, in the
aggregate of several simulations with tracking errors seeded differently, clear patterns of dependency emerge [circles in Fig. 7(a to c)]. In particular, the likelihood of large mass errors:

- increases significantly with increasing tracking errors [Fig. 7(a)] with a quasi-linear variation [Fig. 8(a)];
- decreases significantly with increasing refinement

The results clearly suggest that accurate tracking is necessary to obtain conservative transport solutions. Additional grid refinement and added diffusion reduce, but do not eliminate mass conservation errors due to tracking.

Fig. 9. Mean first moment for 12 seeds (circles and dashed line): (a) vs. $e/\Delta x$; (b) $\sigma/\Delta x$; and (c) $D^*$. 

Fig. 10. Standard deviation of the mean first moment: (a) vs. $e/\Delta x$; (b) $\sigma/\Delta x$; and (c) $D^*$. 

Fig. 11. Potential for instabilities in the presence of tracking errors for a tracking error of 50%: (a) concentration field for time steps 0, 11 and 48; (b) $L_2$-norm for pi-ELM and reference ELM—instability generated by the presence of tracking errors.

The results clearly suggest that accurate tracking is necessary to obtain conservative transport solutions. Additional grid refinement and added diffusion reduce, but do not eliminate mass conservation errors due to tracking.

Fig. 12. Time series of second moment with tracking errors scaled by time series of second moment without tracking errors (both with $Cu = 0.5$).
5.2.3 Phase errors

The dependence of phase errors on the dimensionless numbers \( \frac{\tau}{\Delta x} \), \( \frac{j}{\Delta x} \) and \( D^* \) is also inconclusive within a single simulation [dashed line in Fig. 9(a to c)]. However, in the aggregate of several simulations with tracking errors seeded differently, patterns of dependency emerge [circles in Fig. 9(a to c)]. In particular, the likelihood of large phase errors:

- increases significantly with increasing tracking errors [Fig. 9(a)], with a quasi-linear variation [Fig. 10(a)];
- decreases significantly with increasing refinement up to \( \frac{\tau}{\Delta x} = 15 \), followed by a slight increase for larger values of \( \frac{\tau}{\Delta x} \) [Fig. 9(b) and Fig. 10(b)];
- decreases significantly with the diffusion number up to \( D^* = 1 \), with a quasi-logarithmic variation [Fig. 9(c) and Fig. 10(c)]. For diffusion numbers larger than 1, phase errors present an almost-linear increase. This behavior can be explained by the dependence of phase errors on diffusion observed in the truncation error analysis [first part of eqn (10)]. For \( D^* > 1 \), simulations are diffusion-dominated, and the first term in the first part of eqn (10) becomes negligible relative to the second.

Our analysis suggests that accurate tracking is necessary to prevent large phase shifts of the order of several times the element size. Added diffusion or finer grid resolution do not effectively reduce phase errors.

5.2.4 Numerical diffusion

Unlike mass and phase errors, numerical diffusion is practically independent of the specific distribution of tracking errors, thus allowing estimates on the expected second moment. For several solutions with inexact tracking, the normalized second moment can be smaller than 1 over some periods of time. Therefore, tracking errors can introduce negative numerical diffusion, as pointed out by the truncation error analysis. Time varying, potentially negative, numerical diffusion can lead to an unstable behavior, especially if inherently less diffusive ELMs than our reference method are used. In order to illustrate this possibility, test 1 was repeated, with a tracking error of 50% and a Courant number of 0.5, using a very accurate piecewise ELM. This method, which is unconditionally stable in the absence of tracking errors, is even more severely affected by inexact tracking than the linear interpolation ELM [Fig. 11(a)] and becomes unstable after a short number of time steps [Fig. 11(b)].

Numerical diffusion can also be increased by the presence of tracking errors. However, the numerical diffusion in presence of inexact tracking is of the same order of magnitude of the numerical diffusion without tracking errors and with a Cu of 0.5 [Fig. 6(c)]. Since the effective Courant number is not kept at 1, the observed second moments of concentration are generated both by tracking errors and by the use of a linear interpolator. In order to allow a meaningful comparison between solutions with and without tracking errors, the runs were repeated for Cu = 0.5 (test 1A), which would lead to the maximum numerical diffusion in the absence of tracking errors. The resulting second moment of concentration was then scaled by the second moment in the absence of tracking errors. The final result presented a short number of time steps (Table 5). In general, larger tracking errors lead to an increased numerical diffusion, which can reach significant values: up to three times its value without tracking errors, after a short number of time steps (Fig. 12).

6 FINAL CONSIDERATIONS

This paper addressed the impact of inexact tracking on Eulerian–Lagrangian solutions of the transport equation through a combination of formal analysis and numerical experimentation. The accuracy (Fig. 13) and the stability of ELMs (Fig. 11) were shown to be severely compromised.
by tracking errors, reinforcing the need for an accurate tracking. Different scenarios result from specific tracking errors distributions, thus preventing accurate estimates of the effect of inexact tracking in a real system. Still, some important features can be identified that recommend the use of accuracy controlled tracking techniques:

- In the presence of complex flows, considerable tracking errors can be generated in surface water simulations if low-order tracking methods are used. Conversely, accuracy-controlled techniques allow for very small tracking errors, regardless of the complexity of the flow pattern or the geometry of the domain.
- Increasing tracking errors lead to wider ranges of both mass and phases errors. For large tracking errors, mass imbalances can be quite significant [Fig. 6(a)]. Similarly, large artificial phase shifts, of the order of several times the grid spacing, can be generated.
- Both negative numerical diffusion and excessive positive numerical diffusion can result from the presence of tracking errors. Negative diffusion can lead to instability, in particular when otherwise very accurate ELMs are used. The positive numerical diffusion associated with large tracking errors can be several times larger than that of the linear interpolation ELM, thus severely hampering the accuracy of the simulations and the usefulness of ELMs for practical purposes.
- Large diffusion coefficients and grid refinements, usual ‘fixes’ for numerical problems, may be ineffective for simulations with significant tracking errors. Additional grid refinement and added diffusion tend to reduce mass errors but are unable to fully eliminate them. Phase errors are not consistently reduced by larger plume discretization or larger diffusion coefficients.
- Tracking errors affect both interpolation and integration finite element ELM formulations, even otherwise very accurate methods such as the piecewise ELM9 and the ELLAMs2 (Fig. 14).

Mass imbalances, generated either by a poor tracking or by a nonconservative flow field, limit the use of ELMs for general applications, in particular when transformation processes are present. While tracking errors can be kept at acceptable levels by accuracy-controlled tracking techniques, mass errors from nonconservative flows pose a difficult, and interesting, challenge.

Several solutions, which resort to conservative forms of the transport equation, have been proposed to address this problem. For models that use the nonconservative transport equation, a simple solution is to approximate the neglected continuity equation term. Another solution is the use of an ELLAM formulation with a finite element framework, which has the potential advantage of using, a priori, a conservative form of the transport equation. However, these two alternatives can only address part of the mass problem in ELMs: neither of them can handle the mass errors that result, on an elemental basis, from errors introduced by non-conservative flows on the tracked image of the element.5,15,16

Recently, Eulerian–Lagrangian concepts within a finite volume framework have shown promise for local mass conservation.5,15,18,21,22,23 In particular, the finite volume ELLAM of Healy and Russell22 and the flux-based ELM of Roache23 have been shown to preserve mass globally, even with inexact tracking. However, inexact tracking and nonconservative flow fields will still lead to local mass imbalances and oscillations.

A potentially more robust and complete solution to the mass conservation problem in ELMs may require the use of very fine grids to reduce flow mass errors. Since grid generation is controlled by different processes in flow and transport, separate grids can be used, thus avoiding unnecessary computational effort in the transport simulation. Further research is still necessary, though, to study and compare these different approaches and provide an Eulerian–Lagrangian formulation that guarantees mass conservation.

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APPENDIX A REVIEW OF MODELS TEA–NL AND ELM

The model TEA–NL25,26 solves the fully nonlinear primitive shallow water equations in the frequency domain. The nonlinear terms are treated iteratively and a linear friction term is added to both sides of the momentum equation to provide iterative stability and improve convergence. The governing equations are:

\[
\frac{\partial h}{\partial t} + \frac{\partial (hu)}{\partial x} + \frac{\partial (vh)}{\partial y} = - \frac{\partial}{\partial x}(\eta u) - \frac{\partial}{\partial y}(\eta v) \quad (A1)
\]

\[
\frac{\partial u}{\partial t} + g \frac{\partial h}{\partial x} - fv + \lambda u = \left[ \lambda - c_t \left( u^2 + v^2 \right)^{1/2} \right] u - u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y}
\]

\[
\frac{\partial v}{\partial t} + g \frac{\partial h}{\partial y} + fu + \lambda v = \left[ \lambda - c_t \left( u^2 + v^2 \right)^{1/2} \right] v - u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y}
\]

where \( u \) and \( v \) are the depth averaged components of velocity; \( \eta \) is the surface elevation relative to mean sea level; \( h \) is the depth relative to mean sea level; \( g \) is the acceleration.
due to gravity; $f$ is the Coriolis factor; $c_t$ is the bottom friction coefficient; and $\lambda$ is the linearized friction factor. 

Eqs (A1) are then reduced to their harmonic form by assuming that $\eta$, $u$, $v$ and the right hand side nonlinear terms may be expressed as Fourier series. This leads to $N_t$ sets of time independent equations of the form:

$$iw\hat{\eta}_j + \frac{\partial}{\partial x}(\hat{u}_j h) + \frac{\partial}{\partial y}(\hat{v}_j h) = P_m^{nl}$$

(A2)

$$iw\hat{u}_j + \frac{\partial}{\partial x}(\hat{u}_j h) - f\hat{\eta}_j + \lambda\hat{u}_j = P_m^{nl}$$

$$iw\hat{v}_j + \frac{\partial}{\partial y}(\hat{u}_j h) + f\hat{\eta}_j + \lambda\hat{v}_j = P_m^{nl}$$

where $w_j$ is the $j$th frequency of the spectrum; $\hat{\eta}_j$, $\hat{u}_j$ and $\hat{v}_j$ are the complex elevation and velocity amplitudes of the $j$th component of $\eta(t, u(t)$ and $v(t)$, respectively; $P_m^{nl}$ is the $j$th harmonic component of the continuity equation nonlinear terms; $P_m^{nl}$ and $P_m^{nl}$ are the $j$th harmonic component of the $x$- and $y$-momentum nonlinear terms, respectively; $N_t$ is the number of frequencies and $i = (-1)^{1/2}$. 

Eqn (A2) is spatially discretized using linear finite elements. A weak residual statement is developed by allowing a residual error on the normal flux boundaries and by error terms by combining several ‘trial’ steps, which involve substep. 

The Runge–Kutta methods (RK) eliminate high-order error terms by combining several ‘trial’ steps, which involve substep. If we substitute eqn (B.1) into eqn (B.2) and truncate the series after the second term, we obtain the first-order, one-step backward Euler (BE, Table 2). The multi-step backward Euler improves the accuracy of the BE by dividing the time step in substeps (MSE, Table 2). The tracking in the boundary model to prevent characteristic lines from crossing these boundaries. Rather than stopping the tracking at the boundary, ELA allows the tracking to continue within a small ‘slippery region’ defined as a thin layer along the boundary.

**APPENDIX B TRACKING TECHNIQUES**

Tracking of characteristic lines in transport models requires solving (shown in one-dimension, for simplicity):

$$\frac{dx}{dt} = u,$$  

(B.1)

where $u(x(t))$ is the velocity; $t$ is time; and $x$ is the spatial coordinate.

Several methods have been used in the past to solve eqn (B.1), ranging from low-order backward Euler methods\(^{21,14}\) to the high-order Runge–Kutta methods\(^{12,13}\) (other methods using semi-analytical tracking\(^{46,37}\) have also been proposed, but cannot be applied when velocity components depend on nodal velocities in all coordinate directions). The concept behind the derivation of Euler and Runge–Kutta methods is the same: the numerical solution approximates the exact solution by a Taylor series:

$$x(t^r) = x(t^{r+1}) + \Delta t \frac{dx}{dt} + \frac{\Delta t^2}{2!} \frac{d^2x}{dt^2} + \cdots + \frac{\Delta t^6}{6!} \frac{d^6x}{dt^6}.$$  

(B.2)

where $\Delta t = t^r - t^{r+1}$.

If we substitute eqn (B.1) into eqn (B.2) and truncate the series after the second term, we obtain the first-order, one-step backward Euler (BE, Table 2). The multi-step backward Euler improves the accuracy of the BE by dividing the time step in substeps (MSE, Table 2). The tracking in the MSE is performed by applying the BE sequentially in each substep.

The Runge–Kutta methods (RK) eliminate high-order error terms by combining several ‘trial’ steps, which involve the evaluation of velocity at intermediate points between $t^r$ and $r^{r+1}$. The general expression for RK tracking is:

$$x(t^r) = x(t^{r+1}) + \Delta t \sum_{j=1}^{k} a_j k_j$$

with

$$k_j = u \left( t^{r+1} + c_j \Delta t, x(t^{r+1}) + \Delta t \sum_{m=1}^{k} b_{jm} \xi_m \right)$$  

(B.3)

where $q$ depends on the order of the method and is equal to $6$ for a fifth-order Runge-Kutta method and equal to $4$ for a fourth-order Runge-Kutta. Many sets of the coefficients
average visited element, was evaluated as: $E_a = \sqrt{(x_r - x_f)^2 + (y_r - y_f)^2}$, 
\begin{equation}
E_a = \frac{\sqrt{(x_r - x_f)^2 + (y_r - y_f)^2}}{D_{\text{average}}},
\end{equation}
where $(x_r, y_r)$ and $(x_f, y_f)$ are the release and final locations. $D_{\text{average}}$ is the equivalent diameter of the average visited element.

\begin{equation}
D_{\text{average}} = 2 \times \sqrt{\frac{\sum_{m=1}^{n} A_m}{\pi}}.
\end{equation}

where $A_m$ is the area of each of the $m$ elements visited during the tracking.

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