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Towards Higher Order Discretization Error Estimation by Error Transport using Unstructured Finite-Volume Methods for Unsteady Problems

Gary Yan and Carl Ollivier-Gooch

Department of Mechanical Engineering
The University of British Columbia, Vancouver, BC, Canada

Corresponding author: gary.yan@alumni.ubc.ca

Abstract: A numerical estimation of discretization error for solutions to unsteady model equations in compressible flow is performed using the error transport equation (ETE) on unstructured meshes. We demonstrate the method for unsteady problems as an extension to our previous work on steady problems, where solving the ETE can be more efficient and robust than solving the higher order primal problem. Two methods of computing the time-dependent ETE source term are presented. These schemes are able to produce error estimates that are higher order accurate to the exact error than the primal solution is to the exact solution, when there is sufficient smoothness in the discretization error, which can arise even for unstructured meshes when the discretization in space is to higher order than the discretization in time, a common approach in practice.

Keywords: Discretization Error Estimation, Error Transport, Higher Order Methods, Unstructured Meshes, Finite-Volume Methods

1 Introduction

Error quantification and estimation is an important but sometimes overlooked aspect when using computational methods to understand physical phenomena. The deviations of computed solutions from physical observations can be attributed to two main sources of error: modelling error and numerical error, with the former arising from the inadequacy of the derived mathematical equations to describe the underlying physics, and the latter arising from the inability to solve these equations exactly. In many fluid flow applications, the magnitudes of numerical error are at least as large as those of modelling error. Therefore, in order to reliably estimate the overall error, when using turbulence models for example, one must first be able to accurately estimate and control the numerical error in solving the derived governing equations. An adequate quantification of the numerical errors associated with a certain approximate solution can be useful to demonstrate how accurate the numerical solution is in satisfying the governing equations, much akin to error bars in experiment. In addition to appraising solution accuracy, an accurate estimate of error is also useful in guiding mesh adaptation, as well as improving the solution through defect correction [1].

Of the classifications of numerical error, discretization error, defined as the difference between the exact solution to the partial differential equation (PDE) and the computed solution, is relatively poorly understood and controlled compared to iteration error or round-off error [2]. The scope of the current work will focus specifically on theoretical and heuristic approaches for obtaining an accurate estimate of discretization error for unstructured meshes. We perform single-grid discretization error estimation using the error transport equation (ETE), an auxiliary PDE derived from the primal one. The ETE has a source term which is the residual of the approximate primal solution. Following the approach for structured meshes, the spatial term is estimated by applying the higher order discrete operator on the converged primal solution. For unsteady problems, a time-dependent term also needs to be computed, which is the focus of the current study. For finite-element methods, there is much theoretical foundation for such error estimation methods, as in [3] and more recently in [4], but work on higher order accurate error estimation using the ETE in the literature is lacking for unstructured finite-volume methods. Our objective is to analyze and discern choices of discretization schemes for solving the ETE to obtain higher order accurate estimates for the discretization error on unstructured meshes.

Banks et al. [5] solved the ETE in a structured mesh context, and found that there are many schemes for which combinations of lower order solutions of the primal equation, the ETE, and sufficiently accurate evaluations of the residual source term for the ETE led to a higher order accurate error estimate. The results of [6] demonstrate the application of the ETE to mapped Cartesian meshes, but do not focus on unstructured meshes having geometric features that do not vary smoothly. Solver capability on unstructured meshes is important because more flexibility is possible with complex geometries, which is common for engineering applications. One of the difficulties we encountered for steady problems is the fact that for such meshes, the truncation error, the exact residual source term for the ETE, is asymptotically d orders larger than the discretization error, where d is the highest number of derivatives in the PDE, due to the lack of error cancellation in the discrete scheme, as reported by [7]. A consequence of this in the primal problem is that some schemes on these meshes may be inconsistent in terms of truncation error, but the discretization error may still converge at prescribed order, a phenomenon not observed for uniform meshes. The large amplitude, high frequency noise that is present in the truncation error for unstructured meshes makes it more difficult to estimate this inconsistent term accurately, necessitating more stringent requirements for accurate error estimation than for uniform meshes. These are some of the difficulties we expect to see also for unsteady problems.

We consider multistage, Runge-Kutta type, implicit time integration schemes for their stability properties for stiff problems; other classes such as multistep methods can be used in a similar way. Multistep and multistage methods have their respective advantages and disadvantages. From the point of view of stability, it can be shown that A-stable multistage methods can have arbitrarily high order, whereas this is not the case for multistep methods [8, 9]. However, the number of stages increases quickly for some higher order time discretizations [10]. Furthermore, fully implicit schemes require solutions of larger nonlinear algebraic systems for the stages, in addition to more stringent stability requirements. Because of this, one common approach is to keep a lower order time discretization with a higher order space discretization [11, 12]. Motivated by efficiency advantages of higher order methods for a given level of error or computational budget [13], we still would like to be formally higher order overall, without the need for constructing higher order methods in time, which we hope to achieve with this ETE method.

A common approach in the literature to measure the quality of a discretization error estimate uses what is known as the effectivity index [14]. This quantity is the ratio of the norm of the discretization error estimate to the norm of the exact discretization error, and in the literature, only its convergence to unity is examined as the mesh is refined; this shows only that the discretization error estimate is asymptotically consistent. We focus, rather, on obtaining higher order accurate error estimates, a stronger condition. When used for defect correction, we show that a higher order accurate error estimate is equivalent to a higher order accurate corrected solution, which should be asymptotically more efficient than lower order schemes for a given level of error, as suggested by [13].

A popular alternative to discretization error estimation is output error estimation using adjoint methods, as seen in [15], where an accurate estimate of error is desired in a functional of the solution, such as lift on a surface, determined from the flow variables governed by a physical model. The current discretization error estimation is a promising competitor to adjoint methods, especially when several output functionals are of interest, because one adjoint problem needs to be formed and solved for each functional, whereas the ETE approach yields higher order accurate corrected solution variables, from which any number of functionals can be computed to higher order, agnostic to the choice of functional. Motivating this approach further, the advantages of the ETE approach should be even greater for unsteady problems, because in the adjoint formulation, the entire primal problem needs to be solved and the solution stored at each time step with the adjoint problem solved backwards in time, whereas in estimating discretization error through the ETE, the primal equation and ETE can be solved concurrently up to a time of interest, without the need to store non-local solution information, although detailed efficiency comparisons are deferred for a later study.

2 Methodology

Following the derivation of Banks et al. [5], suppose the governing mathematical model can be written for the solution $\mathbf{u}(\mathbf{x}, t)$ as a conservation law:

$$\partial_t \mathbf{u} + \nabla \cdot \mathbb{F}(\mathbf{u}) = \mathbf{s}(\mathbf{u}), \tag{1}$$

where the solution $\mathbf{u}(\mathbf{x}, t)$ and physical source term $\mathbf{s}$ is in some sufficiently continuous function space $\mathcal{C}(\Omega)$, over a domain $\Omega \subset \mathbb{R}^m \times [0, \infty)$, $\mathbf{x} \in \mathbb{R}^m$. The number of spatial dimensions is $m = 1$, 2, or 3, and $\mathbb{F}$ is the flux dyad in the coordinate directions. In some models such as viscous flows, the flux depends on the gradient of the solution but we only explicitly write this dependence when specifically discussing those models. For ease of representation, the discussion is restricted to $m = 1$, but still considering a system of equations; the multi-dimensional case can be derived similarly. In this case equation (1) becomes

$$\partial_t \mathbf{u} + \partial_x \mathbf{f}(\mathbf{u}) = \mathbf{s}(\mathbf{u}). \tag{2}$$

Let $\tilde{\mathbf{u}}(x, t)$ be a continuous approximation to $\mathbf{u}(x, t)$. The continuous discretization error of interest is then defined as $\mathbf{e}(x, t) := \mathbf{u}(x, t) - \tilde{\mathbf{u}}(x, t)$. Substituting this for $\mathbf{u}(x, t)$ in equation (2), we get

$$\partial_t(\mathbf{e} + \tilde{\mathbf{u}}) + \partial_x \mathbf{f}(\mathbf{e} + \tilde{\mathbf{u}}) = \mathbf{s}(\mathbf{e} + \tilde{\mathbf{u}}). \tag{3}$$

Subtracting the quantity $\partial_t \tilde{\mathbf{u}} + \partial_x \mathbf{f}(\tilde{\mathbf{u}}) - \mathbf{s}(\tilde{\mathbf{u}})$ from both sides, then rearranging, this yields

$$\partial_t \mathbf{e} + \partial_x \left(\mathbf{f}(\mathbf{e} + \tilde{\mathbf{u}}) - \mathbf{f}(\tilde{\mathbf{u}})\right) - \left(\mathbf{s}(\mathbf{e} + \tilde{\mathbf{u}}) - \mathbf{s}(\tilde{\mathbf{u}})\right) \quad = \quad -(\partial_t \tilde{\mathbf{u}} + \boldsymbol{\mathcal{R}}(\tilde{\mathbf{u}})), \tag{4}$$

where $\boldsymbol{\mathcal{R}}(\tilde{\mathbf{u}}) := \partial_x \mathbf{f}(\tilde{\mathbf{u}}) - \mathbf{s}(\tilde{\mathbf{u}})$ is defined as the spatial residual and specifically corresponds to the flux integral for finite-volume methods. We see that the discretization error is governed by a differential operator different than that for the solution, driven by a time-dependent residual of the approximate primal solution. Rather than the full form of the ETE, some simplifications are often used, but this is not considered currently.

2.1 Discretization in space

In this section we discuss our approach to discretizing the problem using the finite-volume method. Integrating the PDE in the form of equation (1) over a control volume Ω_i, $i = 1, ..., M$, and dividing by the volume $|\Omega_i|$, we get

$$\frac{1}{|\Omega_i|} \int_{\Omega_i} \partial_t \mathbf{u} \, d\mathbf{x} + \frac{1}{|\Omega_i|} \int_{\Omega_i} \nabla \cdot \mathbb{F} \, d\mathbf{x} = \frac{1}{|\Omega_i|} \int_{\Omega_i} \mathbf{s} \, d\mathbf{x}. \tag{5}$$

The finite-volume formulation is obtained by applying the divergence theorem, from which the semi-discrete form can be obtained

$$\frac{dU_i}{dt} + \frac{1}{|\Omega_i|} \oint_{\partial \Omega_i} \mathbb{F} \cdot \hat{\mathbf{n}} \, d\sigma = S_i \tag{6}$$

with the upper-case variables denoting averages over the control volume. For the one-dimensional case this reduces to

$$\frac{dU_i}{dt} + \frac{1}{|\Omega_i|} (F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}) = S_i, \tag{7}$$

where $F_{i+\frac{1}{2}}$ and $F_{i-\frac{1}{2}}$ are right and left face flux values for control volume i. Defining the discrete spatial residual as

$$R_i(U) := \frac{1}{|\Omega_i|} (F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}) - S_i, \tag{8}$$

we get the following system of ordinary differential equations (ODEs) for the control volume averages:

$$\frac{dU}{dt} = -R(U) \tag{9}$$

as a method-of-lines type discretization. In the same way, the ETE, equation (4) can be discretized as

$$\frac{d\epsilon}{dt} = -(R(U+\epsilon) - R(U)) + \tau(U) \tag{10}$$

where the terms on the right make up the spatial residual for the ETE. τ is the discrete version of the ETE source term $-(\partial_t \tilde{\mathbf{u}} + \boldsymbol{\mathcal{R}}(\tilde{\mathbf{u}}))$, and ϵ is the discrete version of the discretization error $\mathbf{e}$.

Our approach to obtaining higher order spatial accuracy in the finite-volume method for unstructured meshes uses k-exact least-squares reconstruction, as discussed in [16, 17]. The fluxes can be evaluated at control volume boundaries using appropriate solution and derivative values of the reconstructed polynomial at quadrature points. However, for a particular point on a face, there are different values of the solution and derivatives reconstructed on either side. A unique flux is evaluated as a function of these two sets of values. For advective fluxes, upwinding is applied via Roe's flux difference splitting scheme [18]. For diffusion, an arithmetic average of fluxes on either side is used, with an additional jump term, as in [19], computed as

$$F_J = \alpha \frac{U_L - U_R}{|\mathbf{r}_{ij} \cdot \hat{\mathbf{n}}|} \tag{11}$$

where α is a constant, $\mathbf{r}_{ij}$ is the vector connecting the reference points of the control volumes i and j sharing the face, $\hat{\mathbf{n}}$ is the outward unit normal of that face, and U_L and U_R are solution values on either sides of the face. This couples adjacent control volumes and stabilizes odd-even modes, and is necessary for the stability of second order schemes for viscous fluxes.

This finite-volume reconstruction method shares some similarities with discontinuous Galerkin finite-element schemes, in the sense that functions are constructed cellwise, jump discontinuities exist across faces, and unique values are evaluated as a function of quantities on either side. In particular, the jump term approach is quite similar to penalty schemes for discontinuous Galerkin, as summarized by [20]. There are advantages and disadvantages to our finite-volume method over discontinuous Galerkin, such as requiring fewer degrees of freedom for a given order of accuracy, but with generally wider stencils. A detailed comparison is not attempted here, but can be found in the literature [21].

In space, we can choose separately the discretization order of the primal equation p, the discretization order of the ETE q, and the order r to which the primal solution is reconstructed for residual evaluation. We can also choose the discretization in time used for the primal problem, denoted by p_t. The time discretization for the ETE is selected to be $q_t = p_t$, which should be a good choice, because for discretizations with uniform spacing, higher order can be achieved in this way, so long as the time discretizations satisfies $r_t > p_t$, as seen in the literature for uniform discretization in space. However, from our previous work for steady problems on unstructured meshes, in space $p = q$ is not sufficient and $p < q$ is used for obtaining higher order accurate error estimates. We will refer to the discretization orders by the ordered 4-tuple $(p, q, r; p_t)$. We also fill the ETE arguments with zeros if only the primal problem is solved. For example, solving the primal problem only with a fourth order space discretization with Crank-Nicolson in time is represented by $(4, 0, 0; 2)$.

2.2 Review of results for steady problems

Having previously studied higher order accurate error estimation techniques using the ETE on unstructured meshes for steady problems, we will carry over some of the methodology and considerations to unsteady problems. As a summary of results for steady problems, model PDEs up to the compressible laminar Navier-Stokes equations were considered. We have shown that the linearized ETE along with $p < q = r$ gives an efficient, accurate error estimate. When used for defect correction, the corrected solution is higher order accurate and can be obtained in a much smaller time than solving the higher order primal problem. This approach can also be more robust than solving the higher order primal problem since only lower order problems need to be solved; the higher-order linearized problem is formulated as a single linear algebraic system without pseudo time stepping. In the steady case, $p < q = r$ estimates the part of the ETE exact source term that dominates. As we will see for the unsteady version, it is not as simple to decompose the ETE source term in this way; most terms involve differences of $\mathcal{O}(1)$ quantities.

2.3 Discretization in time

From the method-of-lines discretization in equation (9) and equation (10), we write the ODE system as

$$\frac{dU}{dt} = f(U) \tag{12}$$
$$\frac{d\epsilon}{dt} = g(\epsilon) + T \tag{13}$$

where f and g represent the right hand side flux integrals, and T is an estimate of the ETE source term. We consider two classical implicit Runge-Kutta type schemes for time integration: backward Euler ($p_t = 1$) and Crank-Nicolson ($p_t = 2$). Using uniform time steps, the backward Euler discretization is

$$\begin{aligned} \frac{U^{n+1} - U^n}{k} &= f(U^{n+1}) \\ \frac{\epsilon^{n+1} - \epsilon^n}{k} &= g(\epsilon^{n+1}) + T^{n+1} \end{aligned} \tag{14}$$

and the Crank-Nicolson discretization is

$$\begin{aligned} \frac{U^{n+1} - U^n}{k} &= \frac{1}{2}(f(U^{n+1}) + f(U^n)) \\ \frac{\epsilon^{n+1} - \epsilon^n}{k} &= \frac{1}{2}(g(\epsilon^{n+1}) + g(\epsilon^n)) + \frac{1}{2}(T^{n+1} + T^n) \end{aligned} \tag{15}$$

where the superscript is the quantity evaluated at that time level. In space, we use unstructured meshes because applications often require complex geometries. Such a requirement is not present in the time discretization, hence using uniform time steps is the method of choice. By doing so, smoothness in the error attributed to the time discretization can be preserved.

Our objective is to pick $T^n, n = 0, 1, ..N$ to estimate τ in equation (10) so that the corrected solution $V^n = U^n + \epsilon^n$ is closer than U^n is to $\overline{U}^n$, the exact continuous solution projected onto the discrete space. With $f = f_p, g = g_q = f_q(U + \cdot) - f_q(U)$ as the right hand sides corresponding to order p and q, the corrected solution can be expressed as

$$\frac{V^{n+1} - V^n}{k} = f_q(V^{n+1}) + f_p(U^{n+1}) - f_q(U^{n+1}) + T^{n+1} \tag{16}$$

for backward Euler and

$$\frac{V^{n+1} - V^n}{k} = \frac{1}{2}(f_q(V^{n+1}) + f_q(V^n)) + \frac{1}{2}(f_p(U^{n+1}) + f_p(U^n) - f_q(U^{n+1}) - f_q(U^n)) + \frac{1}{2}(T^{n+1} + T^n) \tag{17}$$

for Crank-Nicolson.

2.4 Accuracy of error estimate

We seek higher order accuracy in the discretization error estimates. For a particular discrete solution to the primal problem accurate to order p, let the exact discretization error on the mesh be ϵ_p, and we wish to estimate this by $\tilde{\epsilon}_p$. If we apply the error estimate as a defect correction, then ensuring higher order accuracy of the corrected solution is equivalent to higher order accuracy of the error estimate, since

$$\overline{U} - (U_p + \tilde{\epsilon}_p) = (\overline{U} - U_p) - \tilde{\epsilon}_p = \epsilon_p - \tilde{\epsilon}_p. \tag{18}$$

In the results to follow, we measure the order of accuracy of the error estimate by computing $\epsilon_p - \tilde{\epsilon}_p$ at the final time as the spatial length scale h and time step k are refined, keeping h/k fixed for each case unless stated otherwise.

2.5 Residual evaluation

The continuous time-dependent residual $-(\partial_t \tilde{\mathbf{u}} + \boldsymbol{\mathcal{R}}(\tilde{\mathbf{u}}))$, the source term for the ETE, is a well-defined quantity, but obtaining an accurate estimate of its discrete analogue is not trivial for unstructured meshes. For the spatial term, $-\boldsymbol{\mathcal{R}}$, Hay and Visonneau [6] discussed several approaches for mapped Cartesian meshes. An obvious method that works well for smooth meshes is to compute the residual by projecting the converged primal solution onto the higher order discrete space. In the current context, we adopt this approach by taking the control volume average of the converged solution of the primal problem, and performing a reconstruction to order r. This yields a piecewise polynomial of degree $r-1$ within each control volume, from which the flux integral can be evaluated. It can be shown that if the ETE source term estimate is within $\mathcal{O}(h^r)$ of the exact ETE source term, then it is sufficient for the discretization error estimate to be within $\mathcal{O}(h^r)$ of the exact error also. However, even for the spatial term, using a reconstruction to order r of the lower order solution does not give an ETE source term that is accurate to $\mathcal{O}(h^r)$ for unstructured meshes. Since the spatial term is investigated in previous studies for steady problems, the focus of the current study is using an estimate T for the time-dependent part of the residual, $-\partial_t \tilde{\mathbf{u}}$. We first start with three pedagogical source terms from which we can hopefully gain some insight. Thereafter, we will discuss the two practical source terms that will be used for the current study.

2.5.1 $T = 0$ gives the trivial zero estimate

In the steady case using $p = r$ leads to this. The error estimate is zero in this case since the ETE source term is zero. To see this, consider the backward Euler discretization, and observe that equation (16) becomes

$$\frac{V^{n+1} - V^n}{k} = f_q(V^{n+1}) + f_p(U^{n+1}) - f_q(U^{n+1}). \tag{19}$$

Clearly $V = U$ is a solution from the backward Euler discretization, hence ϵ is zero.

2.5.2 Source term for exact error estimate

If we impose that $V = \overline{U}$, from equation (16) we have

$$T^{n+1} = \frac{\overline{U}^{n+1} - \overline{U}^n}{k} - f_q(\overline{U}^{n+1}) - f_p(U^{n+1}) + f_q(U^{n+1}) \tag{20}$$

for backward Euler and

$$\frac{T^{n+1} + T^n}{2} = \frac{\overline{U}^{n+1} - \overline{U}^n}{k} + \frac{1}{2}\Big(-f_q(\overline{U}^{n+1}) - f_p(U^{n+1}) + f_q(U^{n+1}) - f_q(\overline{U}^n) - f_p(U^n) + f_q(U^n)\Big) \tag{21}$$

for Crank-Nicolson from equation (17).

2.5.3 Higher order error estimate in space only

For either backward Euler or Crank-Nicolson, using $T^n = f_q(U^n) - f_p(U^n)$ will give higher order accuracy in space only for $q > p$. For example, using $p = 2$, $q = 4$, $p_t = 2$, this gives an identical error in the error estimate as the primal error using $p = 4$, $p_t = 2$, where the time accuracy is unchanged. To see this, equation (17) for the backward Euler discretization becomes

$$\frac{V^{n+1} - V^n}{k} = f_q(V^{n+1}) \tag{22}$$

which means the corrected solution satisfies the space discretization to order q but time accuracy is unchanged. A simple diffusion case is shown using this ETE source term in figure 1. The accuracy of the error estimate versus length scale and time step with k/h^2 fixed is shown in figure 2. It is remarkable, but expected, that the difference of the noisy errors give a smooth profile, which is consistent with the fact that the error in the corrected solution is dominated by the lower order error in the time discretization. If spatial higher order accuracy is sufficient, this method can be used. However, as seen for steady problems, there

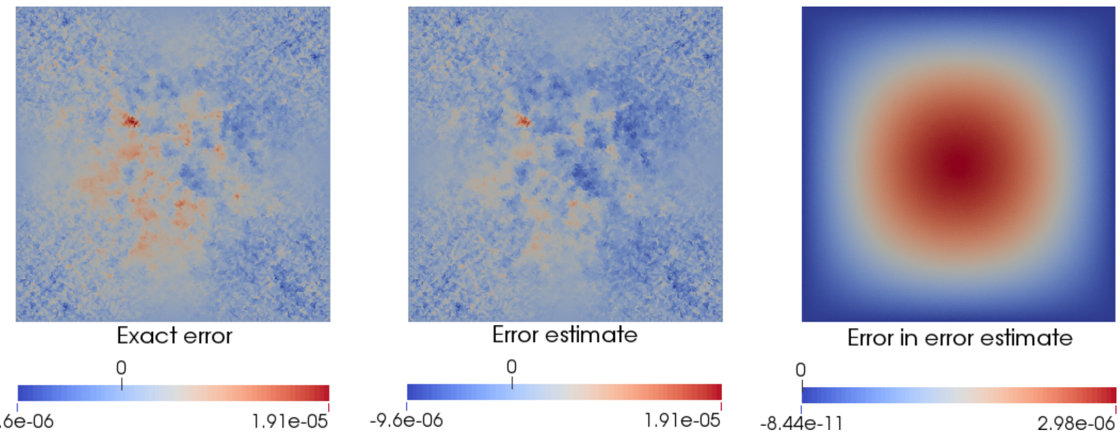


Figure 1: Discretization error, estimate, and difference for a diffusion problem using $(2, 4, 4; 2)$ and $f_q(U) - f_p(U)$ as the ETE source term.

are cost savings over solving only the fourth order primal if we linearize the ETE. There are no apparent advantages here, since a different Jacobian to higher order would need to be computed at each time step if linearization is performed, which would be more expensive than just solving the primal problem to higher order. In contrast for the steady case the Jacobian at the converged solution can be used.

2.5.4 Computing the time derivative $-(\partial_t \tilde{\mathbf{u}} + \boldsymbol{\mathcal{R}}(\tilde{\mathbf{u}}))$ directly

We will show results for the following two methods. As in the steady case, the spatial residual $\boldsymbol{\mathcal{R}}$ is computed using the reconstruction of the primal solution to order r, which is readily computable since solving the primal problem gives the solution at each time step, $U^n, n = 0, 1, ...N$. The time derivative $\partial_t \tilde{u}$ can be computed using a finite difference in time of the primal solution at nearby time steps. For interior nodes in time, D_r, a centered finite difference operator to order r is used:

$$T^{n+1} = -(D_r U^{n+1} + R_r U^{n+1}) \tag{23}$$

where R_r is the spatial residual using a reconstruction of the primal solution to order r, One-sided differences are used in startup and nearing the end time. In the results we will refer to this method as finite difference (FD).

2.5.5 Modified equation analysis

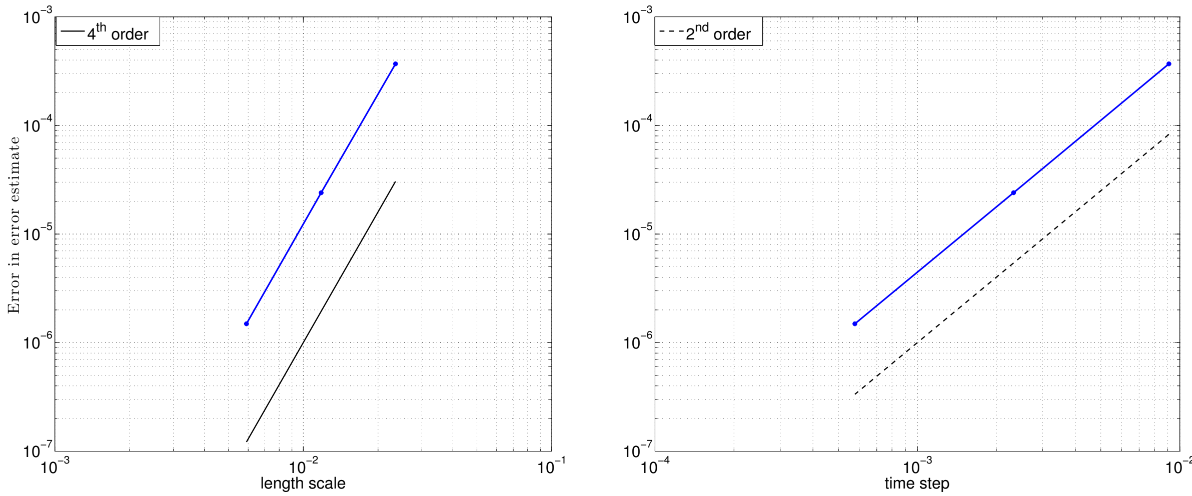
Another approach for the unsteady ETE source term is motivated by modified equation analysis (MEA) [22]. First we observe that the semidiscrete form gives a system of ODEs, equation (12). With sufficient smoothness in the right hand side, for instance when the magnitude of error is dominated by the time discretization with uniform time steps, the standard MEA approach is used to exchange time derivatives in favor of spatial derivatives. For equation (12), the ETE can be derived as

$$\frac{d\epsilon}{dt} = f(U + \epsilon) - f(U) - \left(\frac{dU}{dt} - f(U) \right) \tag{24}$$

which is in the form of equation (13), and U is the fully discrete approximate solution. We start with the backward Euler discretization and expand in a Taylor series about U^n, collecting terms in powers of k. Letting $\mathrm{u} = U^n$, $\mathrm{f} = f(U^n)$, we have

$$\frac{\mathrm{u} + k\mathrm{u}_t + k^2 \mathrm{u}_{tt}/2 - \mathrm{u}}{k} + \mathcal{O}(k^2) = f(\mathrm{u} + k\mathrm{u}_t + \mathcal{O}(k^2)) \tag{25}$$

$$\mathrm{u}_t + \frac{k}{2}\mathrm{u}_{tt} = \mathrm{f} + k\mathrm{f}_\mathrm{u}\mathrm{u}_t + \mathcal{O}(k^2). \tag{26}$$



(a) Versus length scale h.

(b) Versus time scale k.

Figure 2: Accuracy of error estimate versus length scale and time step with k/h^2 fixed during refinement.

From this we know that $\mathrm{u}_t = \mathrm{f} + \mathcal{O}(k)$, and hence $\mathrm{u}_{tt} = \mathrm{f}_t + \mathcal{O}(k) = \mathrm{f}_\mathrm{u}\mathrm{u}_t + \mathcal{O}(k) = \mathrm{f}_\mathrm{u}\mathrm{f} + \mathcal{O}(k)$. Substituting and rearranging, this gives

$$\mathrm{u}_t - \mathrm{f} \quad = \quad \frac{k}{2}(\mathrm{f}_\mathrm{u}\mathrm{f}) + \mathcal{O}(k^2) \tag{27}$$

The ETE source term is then

$$T^{n+1} = -\frac{k}{2}(f_U f)|^{n+1} \tag{28}$$

Alternatively, to see why this particular source term should give a second order correction in time, observe that it is sufficient for the corrected solution to satisfy the Crank-Nicolson discretization

$$\frac{V^{n+1} - V^n}{k} = \frac{1}{2}(f(V^{n+1}) + f(V^n)) \tag{29}$$

From equation (16), this is

$$T^{n+1} = \frac{1}{2}(f(V^n) - f(V^{n+1})) = -\frac{k}{2}(Jf)|^{n+1} + \mathcal{O}(k^2) \tag{30}$$

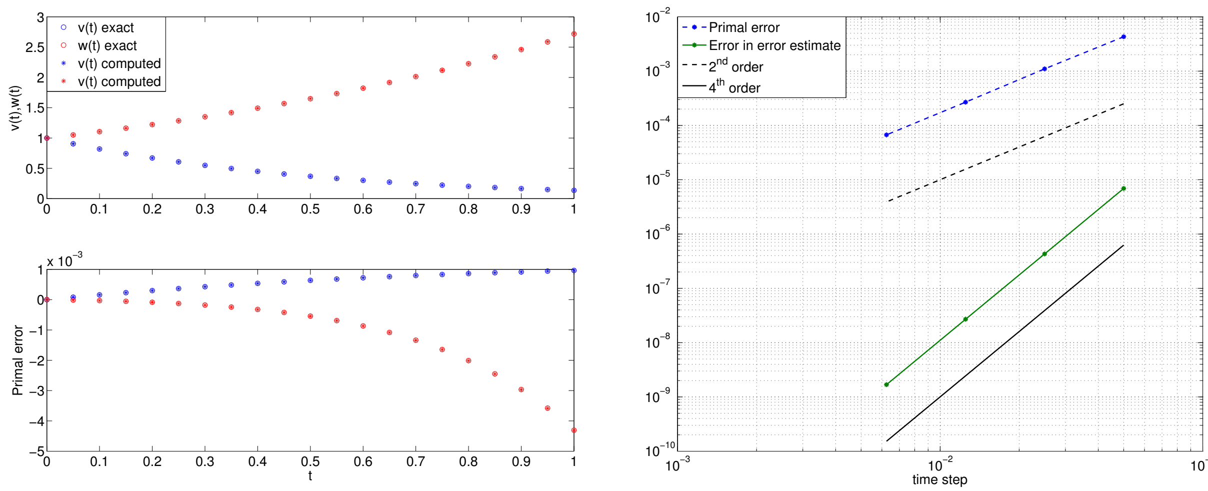
where $J := f_U$ is the Jacobian matrix. Hence using the ETE source term of equation (28) will give second order accuracy in time.

In a similar manner, using Crank-Nicolson it can be shown that

$$\mathrm{u}_t - \mathrm{f} = \frac{k^2}{12}(\mathrm{f}_{\mathrm{uu}}\mathrm{f}^2 + \mathrm{f}_\mathrm{u}^2\mathrm{f}) + \mathcal{O}(k^4) \tag{31}$$

The ETE source term used is thus

$$\begin{aligned} T^{n+1} &= -\frac{k^2}{12}(f_{UU}f^2 + f_U^2 f)|^{n+1} \\ T^n &= -\frac{k^2}{12}(f_{UU}f^2 + f_U^2 f)|^n \end{aligned} \tag{32}$$



(a) ODE system solution and error.

(b) Accuracy of error estimate.

Figure 3: Accuracy of error estimate using the MEA source for a simple ODE system.

There are different ways in computing the term on the right side. One way is to directly compute the Hessian f_{UU}, a third rank tensor, and compute its inner product with f twice. Another way to compute this is to first observe that

$$f_{UU}f^2 + f_U^2 f = (f_U f)_U f. \tag{33}$$

Practically, this can be computed as a Fréchet derivative in the direction f

$$\frac{(Jf)(U + \delta U) - (Jf)(U)}{\delta} f \tag{34}$$

which can be simplified to

$$\frac{(Jf)(U + f(U)\delta) - (Jf)(U)}{\delta} \tag{35}$$

for small $\delta \approx 10^{-8}$.

To demonstrate this method, consider a simple ODE system for $u(t) = [\ v(t) \quad w(t)\ ]^T$

$$\frac{du}{dt} = \frac{d}{dt}\begin{bmatrix} v \\ w \end{bmatrix} = \begin{bmatrix} -2/(uv^4) \\ 1/(uv) \end{bmatrix} \tag{36}$$

with initial conditions $u(0) = [\ 1 \quad 1\ ]^T$. It can be verified that $u(t) = [\ e^{-2t} \quad e^t\ ]^T$ satisfies the ODE system. If sufficient smoothness is assumed, this is in the form of the PDE after finite-volume discretization in space. The ETE is formulated and the ETE source term is computed using the Hessian. It can be seen in figure 3 that the primal solution is second order accurate, and using the proposed ETE source term the error estimate is fourth order accurate, $||u(t = 1) - U(t = 1)|| = \mathcal{O}(k^4)$.

3 Results

We first assume sufficient smoothness in the discretization error, which can arise if the error is dominated by the discretization in time, or $p > p_t$. This is unlike the steady case or when $p \le p_t$, where errors are not smooth. We start with $(4, 2, 4; 2)$ discretizations, where the primal solution is second order accurate overall, and the objective is to get an error estimate that is fourth order accurate overall relative to the exact error.

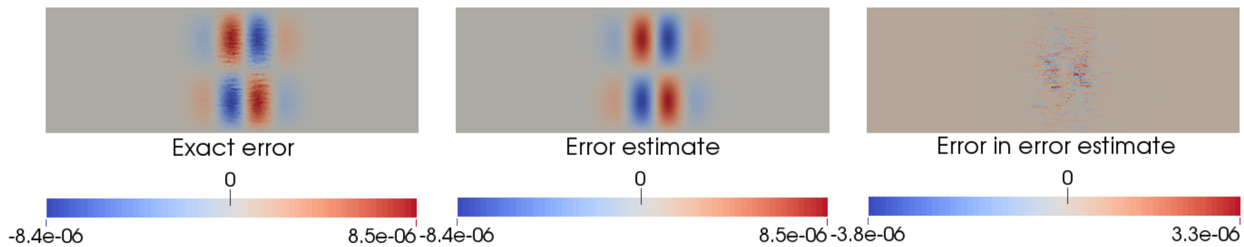


Figure 4: Discretization error, estimate, and difference for the advection problem using $(4, 2, 4; 2)$ FD time derivative ETE source term.

For these cases it was found that q can be decreased to as small as the time discretization without affecting the error estimate accuracy.

3.1 ETE source term by FD

3.1.1 Advection in 2D

We consider the linear advection problem in 2D, as

$$\partial_t u + \mathbf{c} \cdot \nabla u \quad = \quad 0, \text{ on } \Omega = \{(x, y, t) \in [0, L] \times [0, 1] \times [0, 0.1]\} \tag{37}$$

with $\mathbf{c} = \begin{bmatrix} 1 & 0 \end{bmatrix}^T$, initial conditions $u(x, y, 0) = e^{-\frac{(x-L/2)^2}{4\mu^2}} \sin 2\pi y$, wall boundary conditions $u(x, 0, t) = u(x, 1, t) = 0$, and parameters $L = 3, \mu = 0.1$. The exact solution is $u(x, y, t) = e^{-\frac{(x-L/2-t)^2}{4\mu^2}} \sin 2\pi y$, which numerically satisfies the inflow conditions $u(0, y, t) = 0$ to machine precision. Plots of the exact error, estimate, and difference for this case are shown in figure 4.

3.1.2 Diffusion in 2D

Next, we consider diffusion in 2D, as

$$\partial_t u - \partial_x^2 u - \partial_y^2 u \quad = \quad 0, \text{ on } \Omega = \{(x, y, t) \in [0, 1]^2 \times [0, 0.1]\} \tag{38}$$

with Dirichlet boundary conditions $u(x, 0, t) = u(x, 1, t) = u(0, y, t) = u(1, y, t) = 0$. The exact solution is $u(x, y, t) = e^{-2\pi^2 t} \sin \pi x \sin \pi y$. Plots of the exact error, estimate, and difference for this case are shown in figure 5.

3.1.3 Viscous Burgers' equation in 2D

One variant of the viscous Burgers' equation in 2D is posed as

$$\partial_t u + \partial_x \left(\frac{u^2}{2} \right) - \partial_x^2 u + \partial_y u \quad = \quad 0, \text{ on } \Omega = \{(x, y, t) \in [0, 1]^2 \times [0, 0.1]\} \tag{39}$$

with exact solution $u(x, y, t) = 2\pi \frac{\Sigma_{n=1}^{\infty} b_n e^{-n^2\pi^2 t} n \sin n\pi x}{b_0 + \Sigma_{n=1}^{\infty} b_n e^{-n^2\pi^2 t} \cos n\pi x}$ whose coefficients are

$$\begin{aligned} b_0 &= \int_0^1 e^{-\frac{1}{2\pi}(1-\cos \pi x)} dx \\ b_n &= 2 \int_0^1 e^{-\frac{1}{2\pi}(1-\cos \pi x)} \cos n\pi x dx \end{aligned}$$

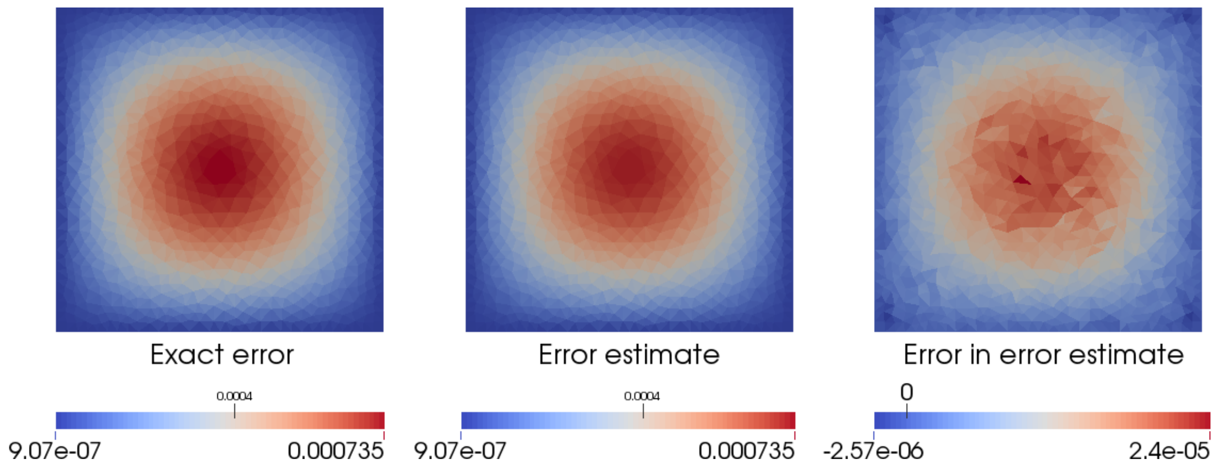


Figure 5: Discretization error, estimate, and difference for the diffusion problem using $(4, 2, 4; 2)$ FD time derivative ETE source term.

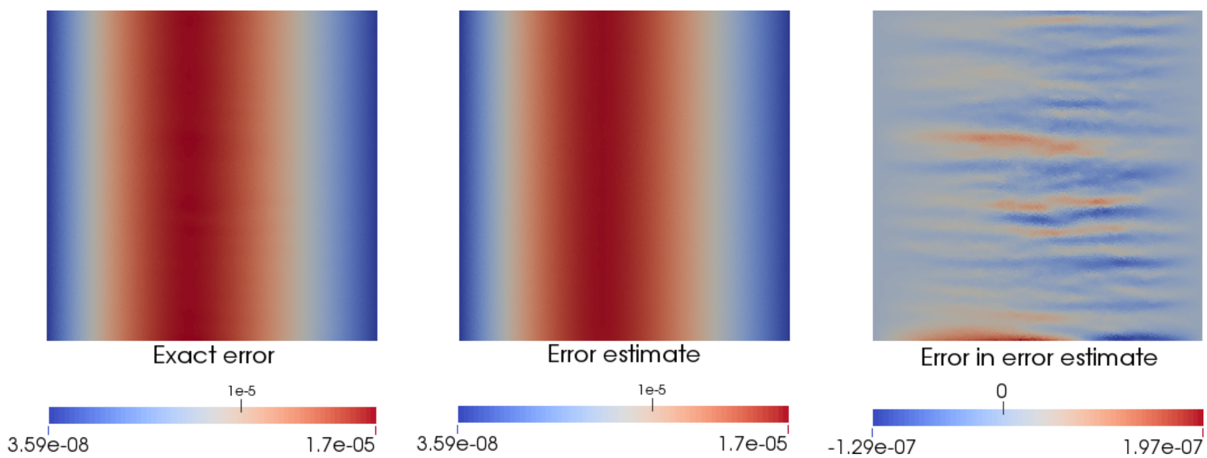


Figure 6: Discretization error, estimate, and difference for the viscous Burgers' equation using $(4, 2, 4; 2)$ FD time derivative ETE source term.

Plots of the exact error, estimate, and difference for this case are shown in figure 6.

3.1.4 Euler equations in 2D

The Euler equations in 2D are

$$\begin{bmatrix} \rho \\ \rho u \\ \rho v \\ E \end{bmatrix}_t + \begin{bmatrix} \rho u \\ \rho u^2 + P \\ \rho u v \\ u(E+P) \end{bmatrix}_x + \begin{bmatrix} \rho v \\ \rho u v \\ \rho v^2 + P \\ v(E+P) \end{bmatrix}_y = \mathbf{0}, \text{ on } \Omega = \{(x, y, t) \in [0, 1]^2 \times [0, 0.1]\} \tag{40}$$

with the vector of conserved variables $\mathbf{u} = \begin{bmatrix} \rho & \rho u & \rho v & E \end{bmatrix}^T$, and an equation of state $P = (\gamma - 1)(E - \frac{1}{2}\rho(u^2 + v^2))$ closes the system. A translating vortex is chosen as an exact solution, computed as

u_∞	v_∞	K	μ	γ	x_0	y_0	ρ_∞	P_∞	a_∞	T_∞
2	2	1	625	1.4	0.4	0.4	1	$1/\gamma$	$\sqrt{\gamma P_\infty/\rho_\infty} = 1$	$1/\gamma$

Table 1: Summary of constants used for the translating vortex test case.

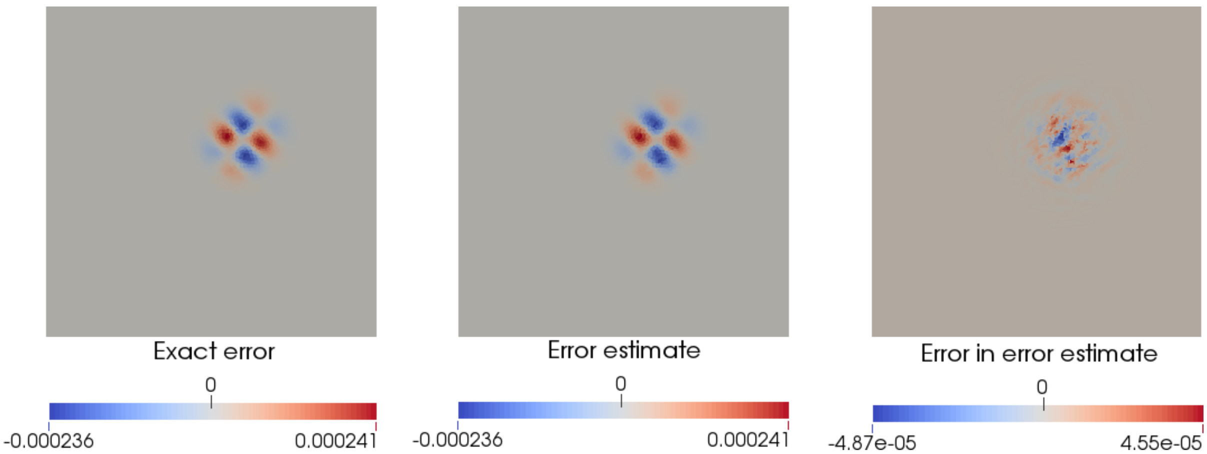


Figure 7: Discretization error, estimate, and difference for the Euler equations using $(4,2,4;2)$ FD time derivative ETE source term.

$$
\begin{aligned}
\frac{u(x,y,t)}{a_\infty} &= \frac{u_\infty}{a_\infty} - \frac{K}{2\pi a_\infty}\bar{y}e^{-\mu\bar{r}/2} \\
\frac{v(x,y,t)}{a_\infty} &= \frac{v_\infty}{a_\infty} + \frac{K}{2\pi a_\infty}\bar{x}e^{-\mu\bar{r}^2/2} \\
\frac{T(x,y,t)}{T_\infty} &= 1 - \frac{K^2(\gamma-1)}{8\pi^2\mu a_\infty^2}e^{-\mu\bar{r}^2} \\
\frac{\rho(x,y,t)}{\rho_\infty} &= \left(\frac{T(x,y,t)}{T_\infty}\right)^{1/(\gamma-1)} \\
\frac{P(x,y,t)}{P_\infty} &= \left(\frac{T(x,y,t)}{T_\infty}\right)^{\gamma/(\gamma-1)}
\end{aligned} \tag{41}
$$

with

$$
\begin{aligned}
\bar{x} &= x - x_0 - u_\infty t \\
\bar{y} &= y - y_0 - v_\infty t \\
\bar{r} &= \left(\bar{x}^2 + \bar{y}^2\right)^{1/2}
\end{aligned} \tag{42}
$$

The non-dimensionalized solution uses the constants shown in table 1. Plots of the exact error, estimate, and difference for this case are shown in figure 7. The accuracy of the primal solution and error estimate for all of these 2D test cases is summarized in figure 8. For each data point, the vertical distance between the primal error and error in the error estimate is a measure of how good the error estimate is, and is also the amount by which the solution will improve if the error estimate is used as a correction, which follows from equation (18). It can be seen that the primal solution is second order accurate, while the error estimate is fourth order accurate.

A more challenging case would be to start with $(2,4,4;2)$, where the discretization error has some noise due to the unstructured discretization in space. The total computational cost for this is approximately the

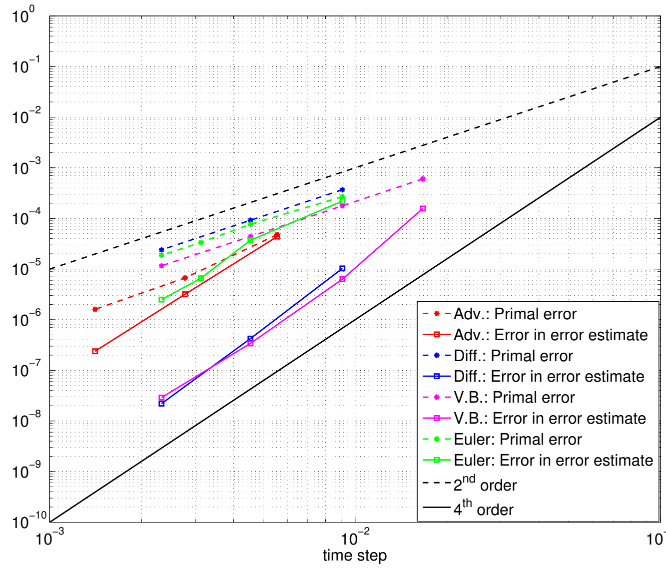


Figure 8: Accuracy of the error estimates using $(4, 2, 4; 2)$ FD time derivative ETE source term.

same as the previous (4,2,4;2) cases. Since both time and space are discretized to the same order, it is expected that this rough nature can be observed in the overall error. For inviscid problems an accurate error estimate can still be obtained, as exemplified by the Euler equations in figure 9, and is quantitatively close to fourth order, as seen in the summary in figure 11. However, for viscous problems the non-smooth nature of the flux integral degrades the result, even though the estimate is qualitatively good, as seen in figure 10 for the diffusion problem. The discretization error in figure 10 is noticeably less smooth than in figure 5, since now the error from the unstructured discretization in space is asymptotically the same as the smooth error from the time discretization.

3.2 ETE source term by MEA

Following the same approach of $p > p_t$ as before, we present results using the MEA source term for the ETE. For $(4, 2, 4; 2)$ the performance is similar to FD for inviscid problems, such as the Euler equations shown in figure 12. The accuracy of the error estimate for the same test cases as before is summarized in figure 13, and we see that fourth order accuracy is achieved for the inviscid test cases.

Again for viscous problems, the non-smooth nature of the repeated application of the flux integral makes the error estimate not smooth, as seen for the diffusion equation in figure 14, and its accuracy degraded in figure 13 to only second order. This is not a problem for lower order discretizations such as $(2, 2, 2; 1)$, whose smoothness can be seen in figure 16, and second order accuracy from a first order time discretization in figure 15. For viscous problems, the spatial discretizations must be at least two, since reconstructing constants ($q = 1$) does not give meaningful gradients. The MEA ETE source term cannot capture the roughness correctly either when $p \leq p_t$, such as the $(2, 4, 2; 2)$ case, as seen in figure 17. This can be compared to the FD ETE source term in figure 10.

4 Conclusion

We have applied the ETE to obtain higher order accurate estimates of discretization error for finite-volume methods on unstructured meshes for some unsteady model problems, using two methods to estimate the time-dependent ETE source term. The FD method computes the time derivative in the time-dependent ETE source term using finite difference of the primal solution, and the MEA method approximates the

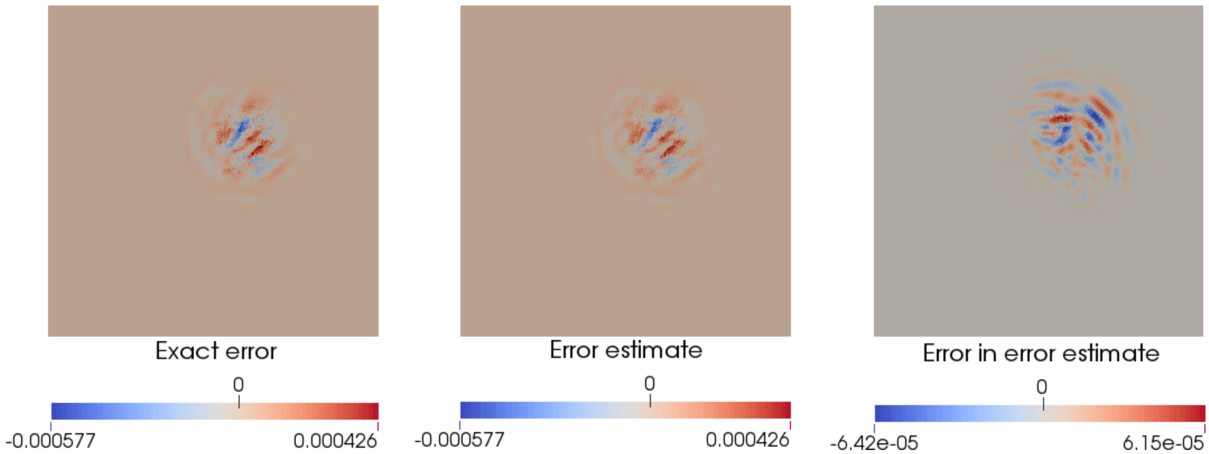


Figure 9: Discretization error, estimate, and difference for the Euler equations using $(2,4,4;2)$ FD time derivative ETE source term.

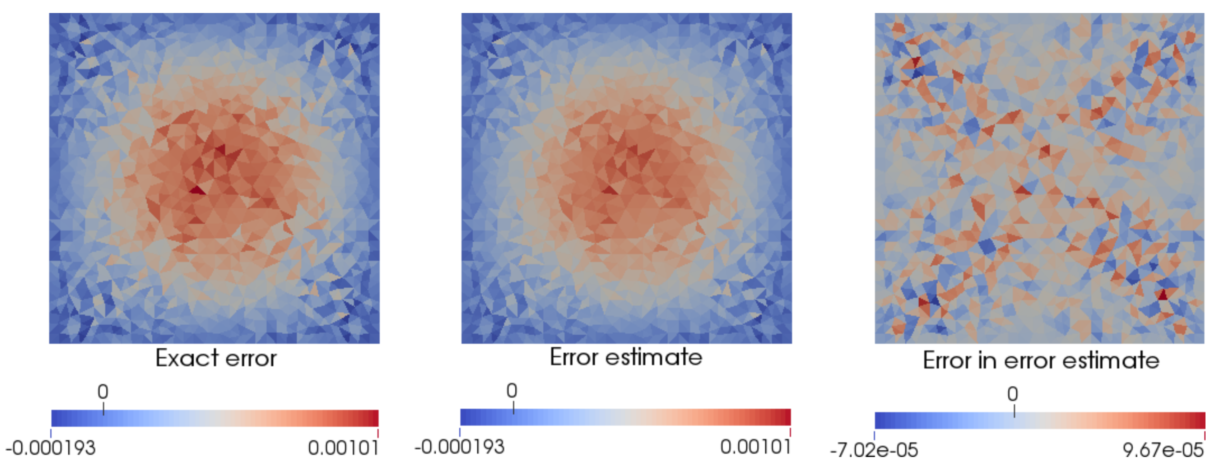


Figure 10: Discretization error, estimate, and difference for the diffusion problem using $(2,4,4;2)$ FD time derivative ETE source term.

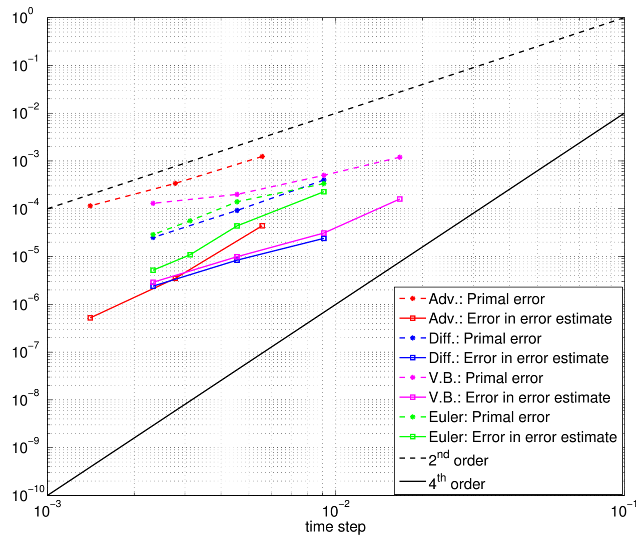


Figure 11: Accuracy of the error estimates using $(2,4,4;2)$ FD time derivative ETE source term.

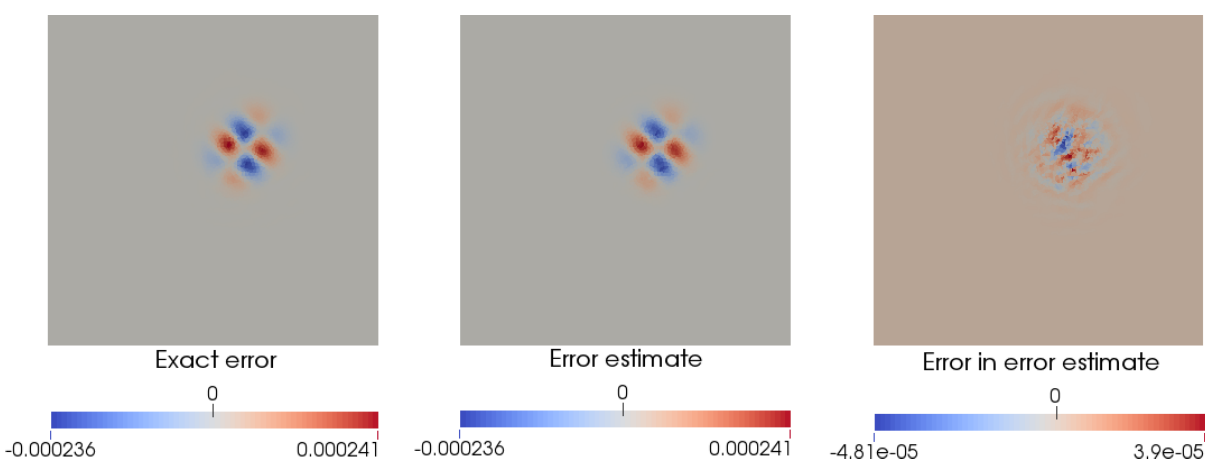


Figure 12: Discretization error, estimate, and difference for the Euler equations using $(4,2,4;2)$ MEA ETE source term.

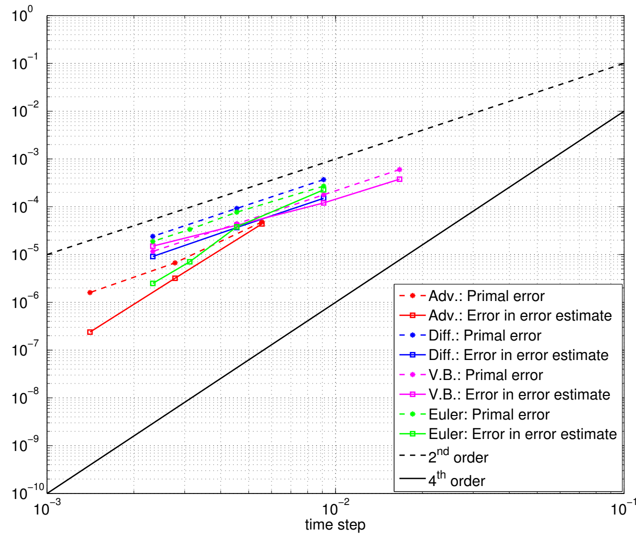


Figure 13: Accuracy of the error estimates using $(4, 2, 4; 2)$ MEA ETE source term.

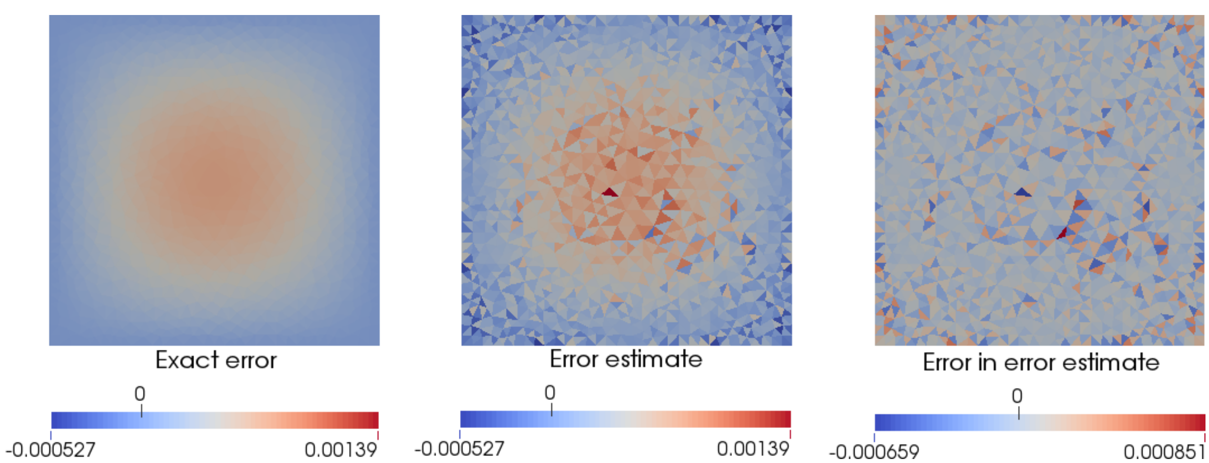


Figure 14: Discretization error, estimate, and difference for the diffusion problem using $(4, 2, 4; 2)$ MEA ETE source term.

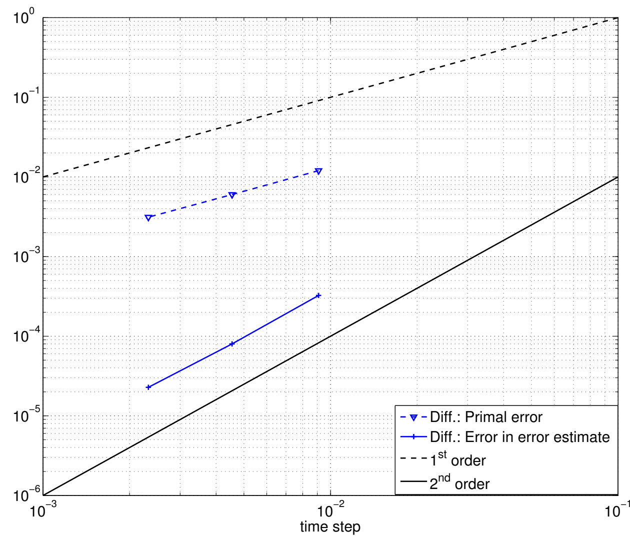


Figure 15: Accuracy of the error estimates using $(2, 2, 2; 1)$ MEA ETE source term for the diffusion problem.

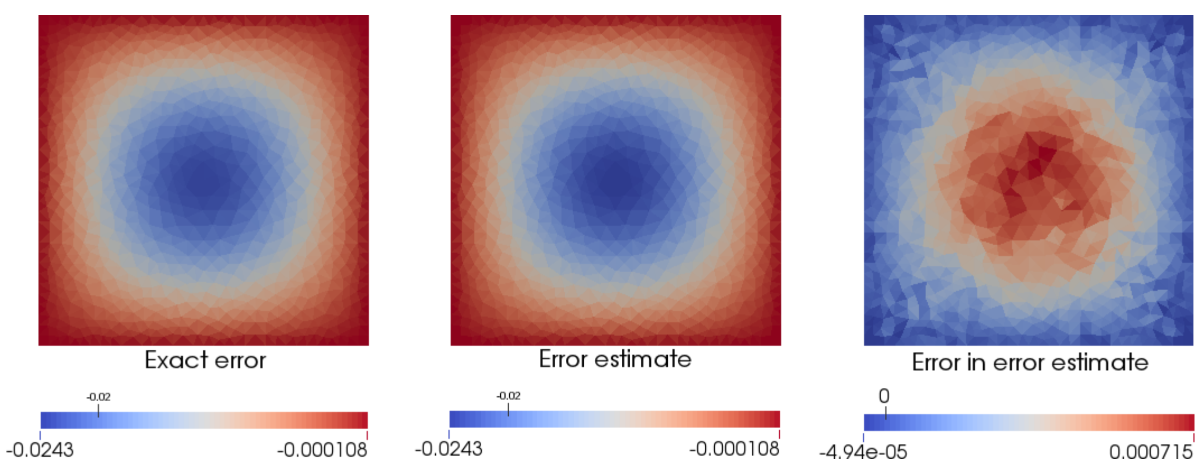


Figure 16: Discretization error, estimate, and difference for the diffusion problem using $(2, 2, 2; 1)$ MEA ETE source term.

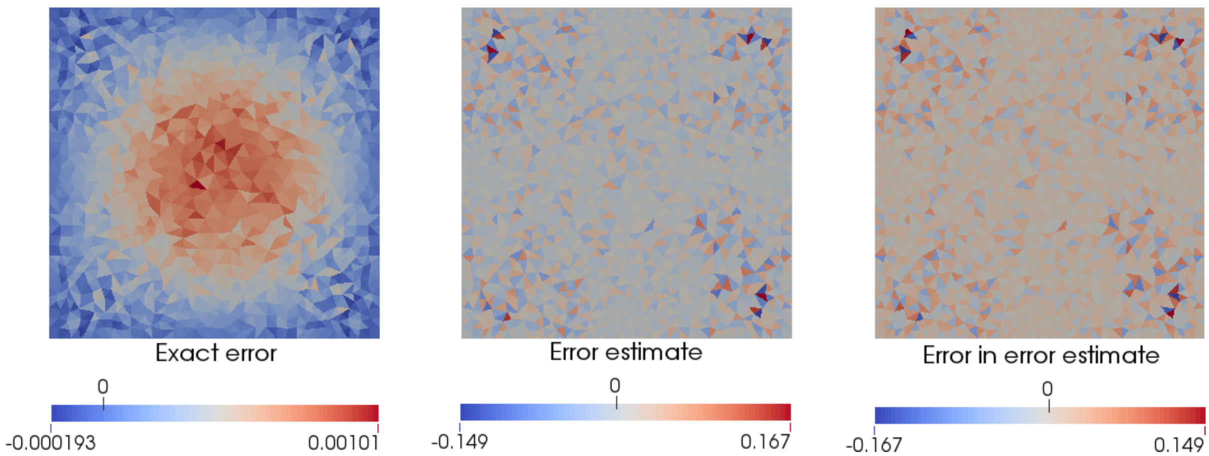


Figure 17: Discretization error, estimate, and difference for the diffusion problem using $(2, 4, 2; 2)$ using MEA ETE source term.

next order terms arising in the method-of-lines discretization. Using a spatial discretization that is higher order than the time discretization in the primal problem, the FD method produces a higher order accurate error estimate from a lower order primal discretization in time across all test cases, while the MEA method produces similar results, but the additional derivative for viscous problems degrades the accuracy of the error estimate. For inviscid models, the FD method can also get accurate error estimates even when the primal problem is discretized to the same order in space and time, where the exact discretization error is not smooth.

For further work, we can investigate the efficiency and robustness properties of this method of error estimation once schemes that perform well are better understood. For these two ETE source terms, both are local in time in the sense that solutions for only a few time steps nearby are required. To reduce the memory footprint, the primal equation and ETE can be co-evolved in time so that the entire solution history does not need to be stored. As in the steady case in previous works, a useful comparison would be against the fully higher order primal problem in space and time. It was found for the steady case that solving a higher order linearized ETE is more efficient and more robust than solving the higher order primal problem. As we have seen, in the unsteady case there are different requirements and different candidate schemes for the ETE that perform well. As an application, we can furthermore perform a detailed comparison of the ETE method against unsteady adjoint methods for output functionals, which should prove to be insightful for practical engineering applications.

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