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A Posteriori Analysis for Hydrodynamic Simulations Using Adjoint Methodologies

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A POSTERIORI ANALYSIS FOR HYDRODYNAMIC SIMULATIONS USING ADJOINT METHODOLOGIES FY08 LDRD FINAL REPORT, 08-FS-005*

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Abstract. This report contains results of analysis done during an FY08 feasibility study investigating the use of adjoint methodologies for *a posteriori* error estimation for hydrodynamics simulations. We developed an approach to adjoint analysis for these systems through use of modified equations and viscosity solutions. Targeting first the 1D Burgers equation, we include a verification of the adjoint operator for the modified equation for the Lax-Friedrichs scheme, then derivations of an *a posteriori* error analysis for a finite difference scheme and a discontinuous Galerkin scheme applied to this problem. We include some numerical results showing the use of the error estimate. Lastly, we develop a computable *a posteriori* error estimate for the MAC scheme applied to stationary Navier-Stokes.

1. Introduction. The adjoint-based approach to *a posteriori* analysis of the effects of perturbation and error on solutions of differential equations uses the adjoint operator to determine the global effects of the local introduction of error. The solution of the adjoint operator carries the stability information that allows an accurate quantification of the effects of propagation, accumulation, and cancelation of perturbations [7]. A key issue with using adjoint-based analysis for nonlinear differential equations is defining the correct adjoint [11, 6]. In general, there are multiple possibilities for a nonlinear problem.

In recent years, there has been significant progress in the analysis of properties of solutions of nonlinear conservation laws using the viscosity solution method, which employs the adjoint operator associated to the stabilized version of the conservation law provided by a vanishing viscosity term [4, 2, 3]. This analysis has established existence, uniqueness, and smoothness properties of solutions by means of properties of the adjoint operator. The stabilized version of the problem is associated with a unique adjoint operator, so in this sense, we can think of the adjoint operator of the stabilized problem as the "right" adjoint operator for treating the stability properties of the solution of the original conservation law.

These observations are particularly relevant for numerical methods for hydrodynamic simulations that depend on some kind of stabilization procedure. In this case,

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the stabilization procedure affects the definition of the correct adjoint operator that should be associated with the numerical method. Moreover, this operator may or may not be particularly close to the adjoint operator associated with the viscosity solution of the problem. We investigate the connection between a numerical method, and any stabilization procedure, and the definition of an adjoint operator that is useful for *a posteriori* error analysis. The goal is to consider how the definition of the adjoint operator reflects the stability properties of the numerical solution. In this work, we explore the definition and use of adjoint operators for error and perturbation analysis for the numerical solution of hydrodynamic properties. We pursue two independent approaches.

First, we consider the problem of defining the correct adjoint operator for a numerical scheme that includes stabilization. As a first step, we consider the classic method of the modified equation for the analysis of a numerical method [12]. The modified equation associated with a numerical method for a differential equation is a new differential equation that has the property that the numerical approximation is a better approximation of the solution of the modified equation than of the original equation. A natural idea is to use the adjoint operator for the modified equation as the adjoint operator for the numerical method.

We undertook to address two questions that arise in this approach:

- Can we identify the adjoint for the modified equation for a numerical method as a reasonable candidate to be the adjoint for the numerical scheme?
- Can we use the adjoint of the modified equation for error analysis?

We carry out this investigation for the Lax-Friedrichs scheme.

Our second approach to using adjoint operator-based error analysis for hydrodynamic simulations is to pursue the extension of the analysis to a stable and accurate finite-volume scheme for the Navier-Stokes equations. We consider the so-called MAC scheme [9, 10], which along with closely related variations, is well-used in the Department of Energy Laboratories. The technical issue here is that the *a posteriori* error analysis is typically applied only to finite element methods, whereas the usual presentation of a finite volume method lacks the variational formulation that is necessary for the use of the adjoint operator. Following [8], we reformulate the MAC scheme as a mixed finite element method with a special quadrature, and then apply the *a posteriori* analysis to this new formulation.

This report is organized as follows. The next section introduces the idea of defining an adjoint operator for a numerical scheme applied to a conservation law by using the viscosity solution and modified equation. Section 3 verifies the adjoint equation to the modified equation for the Lax-Friedrichs scheme applied to Burger's equation. Section 4 derives *a posteriori* error analysis for a finite difference scheme and a discontinuous Galerkin scheme equivalent to the Lax-Friedrichs method and presents some numerical results. Section 5 derives a computable *a posteriori* error estimate for the MAC scheme applied to stationary Navier-Stokes. The last section makes some conclusions.

2. Defining adjoint operators using the viscosity solution and the modified equation.

An important issue for *a posteriori* analysis is defining the appropriate adjoint operators for both the original problem and its discretizations. For nonlinear problems in general, there is not a unique definition, see[11]. In addition, discretization issues, such as stabilization, may also affect the definition of an adjoint operator.

For the conservation law, we propose to use the adjoint operator associated with the vanishing viscosity solution. Suppose u denotes the solution of the conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0. \tag{2.1}$$

We set $A(u) = f'(u)$ and for small $\epsilon > 0$, we let u_ϵ solve

$$\frac{\partial u_\epsilon}{\partial t} + A(u_\epsilon)\frac{\partial u_\epsilon}{\partial x} = \epsilon \frac{\partial^2 u_\epsilon}{\partial x^2}. \tag{2.2}$$

Note that we are ignoring boundary conditions in the discussion below and we assume that appropriate boundary conditions are imposed on the solution. In practice, it is important to consider the boundary conditions when defining adjoint operators.

The solution u_ϵ is the *vanishing viscosity* solution. The introduction of the diffusion term stabilizes the problem, which makes it possible to prove strong properties for u_ϵ. Moreover, we can prove that u_ϵ converges to the physically meaningful (entropy decreasing) solution u of (2.1) and subsequently deduce properties of the solution u. This analysis uses the adjoint problem

$$-\frac{\partial \eta_\epsilon}{\partial t} - A(u_\epsilon)^* \frac{\partial \eta_\epsilon}{\partial x} = \epsilon \frac{\partial^2 \eta_\epsilon}{\partial x^2} \tag{2.3}$$

that can be associated with (2.2) in a natural way.

To determine an adjoint for a numerical method, we consider the method of the modified equation. A modified equation for a numerical method for a given differential equation is another differential equation that the numerical scheme approximates the solution of with higher accuracy than it approximates the solution of the original problem. Typically, the modified equation can be identified through a Taylor approximation analysis and is obtained by adding higher order derivative terms with coefficients depending on the discretization parameters to the original equation.

We consider the linear version of Burgers equation,

$$u_t + au_x = 0. \tag{2.4}$$

We construct a discrete grid $\{x_j, t_n\}$ in space-time, with spacing h and k in space and time respectively. The explicit upwind scheme is

$$\frac{U_j^{n+1} - U_j^n}{k} + c\frac{U_j^n - U_{j-1}^n}{h} = 0. \tag{2.5}$$

We define the truncation error

$$\epsilon_j^n(u) = u_j^{n+1} - u_j^n + \eta(u_j^n - u_{j-1}^n), \quad \eta = ck/h.$$

Using Taylor's theorem, it is straightforward to show that the truncation error satisfies

$$|\epsilon_j^n(u) - k(u_t(x_j, t_n) + au_x(x_j, t_n)) = \mathbf{O}(k^2, kh).$$

If we let w solve the modified equation

$$w_t + aw_x = \frac{ah}{2}\left(1 - \frac{ak}{h}\right) w_{xx} \tag{2.6}$$

then

$$\left|\epsilon_j^n(w) - k\left(w_t(x_j,t_n) + aw_x(x_j,t_n) - \frac{ah}{2}\left(1-\frac{ak}{h}\right)w_{xx}\right)\right| = \mathbf{O}(k^3, kh^2).$$

In other words, U is a closer approximation of w than of the original solution u.

For the Lax-Friedrichs scheme,

$$U_j^{n+1} = \frac{1}{2}(U_{j-1}^n + U_{j+1}^n) - \frac{k}{2h}a(U_{j+1}^n - U_{j-1}^n) = 0, \tag{2.7}$$

the modified equation is

$$w_t + aw_x = \frac{h^2}{2k}\left(1-\left(\frac{ak}{h}\right)^2\right)w_{xx}. \tag{2.8}$$

The modified equation for the Lax-Wendroff scheme for (2.4) is

$$w_t + aw_x = \frac{h^2 a}{6}\left(\frac{a^2k^2}{h^2} - 1\right)w_{xxx}. \tag{2.9}$$

The modified equation for the Beam-Warming scheme for (2.4) is

$$w_t + aw_x = \frac{h^2 a}{6}\left(\frac{ak}{h} - 1\right)\left(\frac{ak}{h} - 2\right)w_{xxx}. \tag{2.10}$$

We show some solutions in Fig. 2.1.

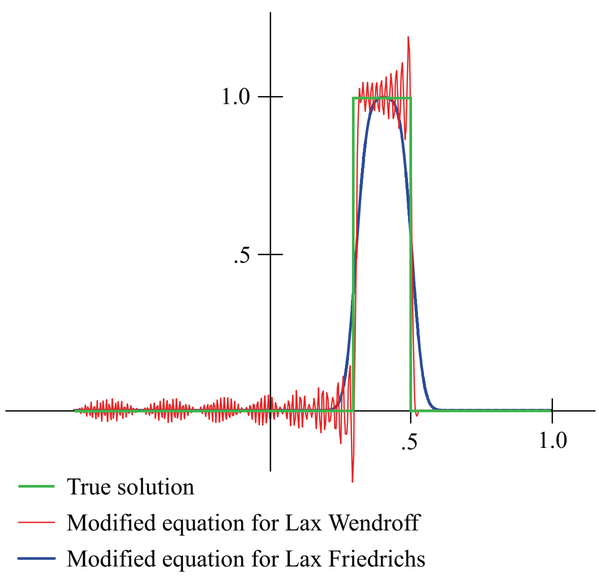

Fig. 2.1: Plots of the solutions of transport equation, the modified equation for the Lax-Friedrichs scheme (2.8), and the modified equation for the Lax-Wendroff scheme (2.9). The initial data is a pulse of height 1 located in $[-.3, 0]$, the transport coefficient $a = 1$, and the solutions are shown at time .5.

We suggest that the adjoint operator corresponding to the modified equation is a natural choice for an adjoint operator for the corresponding difference scheme. For example, we use

$$-\phi_t - a\phi_x = \frac{h^2}{2k}\left(1 - \left(\frac{ak}{h}\right)^2\right)\phi_{xx} + \psi \tag{2.11}$$

as the adjoint operator for the Lax-Friedrichs scheme. For the Lax-Wendroff scheme, we propose

$$-\phi_t - a\phi_x = \frac{h^2 a}{6}\left(\frac{a^2k^2}{h^2} - 1\right)\phi_{xxx} + \psi. \tag{2.12}$$

For data, we choose $\psi = 1/T$ where T is the final time of computation while the "initial" data for the adjoint problem posed at time T is 0. This corresponds to choosing

$$\frac{1}{T}\int_0^T \int_{-\infty}^{\infty} u(t,x)\,dxdt, \tag{2.13}$$

as the quantity of interest. We show adjoint solutions in Fig. 2.2. The differences in the stability properties of the two problems corresponding to Lax-Friedrichs and Lax-Wendroff is evident.

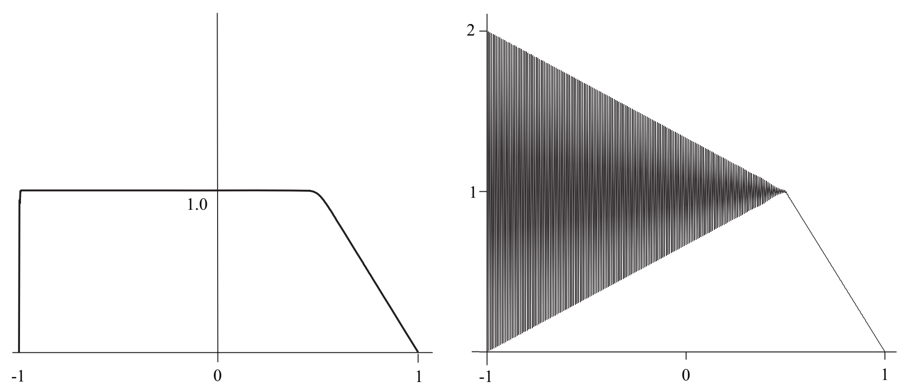

Fig. 2.2: Right: A solution of the adjoint equation for Lax-Friedrichs. Left: A solution of the adjoint equation for Lax-Wendroff. The adjoint data is $\psi = 1$, the transport coefficient $a = 1$, and the solutions are shown at time .5.

Alternatively, we can specify

$$\int_{-\infty}^{\infty} u(T,x)\,dx \tag{2.14}$$

as the quantity of interest by choosing $\psi = 0$ and setting the initial data for the adjoint problem at time T to be 1. We show a solution in Fig. 2.3.

3. Verifying the adjoint equation for the modified equation. In this first calculation, we verify that (2.11) is the correct adjoint for the modified equation (2.8)

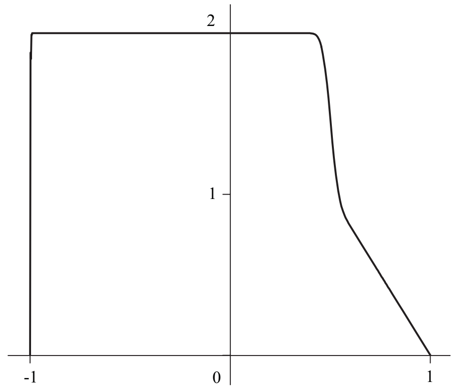

Fig. 2.3: A solution of the adjoint equation for Lax-Friedrichs corresponding to a quantity of interest at the final time $T = .5$.

for the Lax-Friedrichs scheme applied to Burger's equation. Analogous computations hold for other difference schemes. We set

$$c(h,k) = \frac{h^2}{2k}\left(1 - \left(\frac{ak}{h}\right)^2\right)$$

so that (2.11) becomes

$$-\phi_t - a\phi_x = c(h,k)\phi_{xx} + \psi. \tag{3.1}$$

We assume that $\tilde{u}$ denotes a solution of a problem obtained from (2.8) by small perturbations of the coefficients. We let $\tilde{w} = \tilde{u} - u$ denote the error. Because the problems are linear and the residual of u is zero, we have

$$\tilde{w}_t + a\tilde{w}_x - c(h,k)\tilde{w}_{xx} = \tilde{R}_{\tilde{u}}(x,t),$$

where we assume that the residual $\tilde{R}_{\tilde{u}}$ is small. Integrating, we have

$$\int_0^T \int_{-\infty}^{\infty} \tilde{R}_{\tilde{u}}(x,t)\phi(x,t)\,dxdt = \int_0^T \int_{-\infty}^{\infty} \big(\tilde{w}_t + a\tilde{w}_x - c(h,k)\tilde{w}_{xx}\big)\phi\,dxdt.$$

We integrate by parts in each term,

$$\int_0^T \int_{-\infty}^{\infty} \tilde{w}_t\phi\,dxdt = \int_{-\infty}^{\infty} \big(\phi(T)\tilde{w}(T) - \phi(0)\tilde{w}(0)\big)\,dxdt - \int_0^T \int_{-\infty}^{\infty} \phi_t\tilde{w}\,dxdt.$$

Since $\phi(T) = 0$ and assuming that the initial error of the perturbed solution is zero, $\tilde{w}(0) = 0$, the boundary terms vanish. Similarly, assuming that $\phi \to 0$ as $x \to \pm\infty$,

$$\int_0^T \int_{-\infty}^{\infty} a\tilde{w}_x\phi\,dxdt = -\int_0^T \int_{-\infty}^{\infty} a\tilde{w}\phi_x\,dxdt.$$

Assuming in addition that $\tilde{w} \to 0$ as $x \to \pm\infty$,

$$\int_0^T \int_{-\infty}^{\infty} c\tilde{w}_{xx}\phi \, dxdt = \int_0^T \int_{-\infty}^{\infty} c\tilde{w}\phi_{xx} \, dxdt.$$

We obtain

$$\int_0^T \int_{-\infty}^{\infty} \tilde{R}_{\tilde{u}}(x,t)\phi(x,t) \, dxdt = \int_0^T \int_{-\infty}^{\infty} \big(-\phi_t - a\phi_x - c(h,k)\phi_{xx} \big) w \, dxdt.$$

Using (3.1), we conclude

THEOREM 3.1. *Let $\tilde{u}$ denote a perturbed solution of the modified equation for the Lax-Friedrichs method, $\tilde{R}_{\tilde{u}}$ denote its residual, ϕ denote the solution of the adjoint problem associated with the modified equation. Then*

$$\int_0^T \int_{-\infty}^{\infty} (\tilde{u} - u) \, dxdt = -\int_0^T \int_{-\infty}^{\infty} \tilde{R}_{\tilde{u}}\phi \, dxdt. \tag{3.2}$$

For the alternate quantity of interest (2.14), we have

$$\int_{-\infty}^{\infty} (\tilde{u} - u)(T,x) \, dx = -\int_0^T \int_{-\infty}^{\infty} \tilde{R}_{\tilde{u}}\phi \, dxdt. \tag{3.3}$$

These are the expected error representation formulas and this shows that we have defined the correct adjoint.

We use the fact that the differential equation is linear and the scheme is translation invariant. The analysis is more complicated for a nonlinear problem. We again form the error $\tilde{w}$, but now we evaluate the residual using linearization. The difference scheme is not translation invariant in general, so $c = c(u)$, and this has to be included in the integration by parts.

4. An *a posteriori* analysis using adjoint operators.

4.1. Direct *a posteriori* analysis for a finite difference scheme. Adjoint-based *a posteriori* analysis is generally applied to finite element methods because it uses variational analysis. Typically, applications to a finite difference methods are carried out by first recasting the finite difference scheme as a finite element method with quadrature to evaluate the integrals. We provide an example of this approach in Sec. 5 below. In this section, we explore a direct application of adjoint-based *a posteriori* analysis to finite difference schemes using the modified equations discussed in Sec. 3.

The idea is based on the use of the modified equation for accuracy analysis. The solution of the modified equation for a difference scheme has the property that its local truncation error is higher order than the truncation error of the solution of the original problem. From the higher order truncation error, we can prove that the difference scheme better approximates the solution of the modified equation than the solution of the original problem. Our conjecture is that the residual of a finite difference scheme in its modified equation is higher order than its residual in the original problem. This makes it natural to use the adjoint of the modified equation for *a posteriori* analysis of the finite difference scheme.

To make this concrete, we have to define the residual of a finite difference approximation. The residual is obtained formally by substituting the approximation into the weak form of the differential equation. To make this substitution, we define a function that interpolates the values of the finite difference scheme.

For the Lax-Friedrichs scheme, we first recognize the weak form of the error representation (3.2),

$$\int_0^T \int_{-\infty}^{\infty} \tilde{R}_{\tilde{u}} \phi \, dxdt = \int_0^T \int_{-\infty}^{\infty} \big(-\phi_t - a\phi_x \big) \tilde{u} \, dxdt + \int_0^T \int_{-\infty}^{\infty} c(h,k) \phi_x \tilde{u}_x \, dxdt. \quad (4.1)$$

We let U denote the piecewise linear, continuous function that interpolates the values of the Lax-Friedrichs approximation U_j^n. This function has sufficient regularity to be substituted directly into (4.1) and its residual resembles the residual of the standard finite element approximation of the modified equation. Given the close connection between the residual of U and the truncation error, we assume that

$$\int_0^T \int_{-\infty}^{\infty} \tilde{R}_U \phi \, dxdt = \mathbf{O}(k^2, kh).$$

We assume that the quantity of interest is (2.14). We begin the error analysis by decomposing

$$\begin{aligned} \int_{-\infty}^{\infty} (U-u)(T,x) \, dx &= \int_{-\infty}^{\infty} (U-w)(T,x) \, dx + \int_{-\infty}^{\infty} (w-u)(T,x) \, dx, \\ &= I + II, \end{aligned} \quad (4.2)$$

where recall that w solves the modified equation (2.8). Applying (3.2) to U gives

$$I = \int_{-\infty}^{\infty} (U-w)(T,x) \, dx = \int_0^T \int_{-\infty}^{\infty} \tilde{R}_U \phi \, dxdt = \mathbf{O}(k^2, kh).$$

Expression II measures the impact of the difference between the solution of the original problem and the modified equation. In order to estimate this term, we decompose it as

$$\begin{aligned} \int_{-\infty}^{\infty} (w-u)(T,x) \, dx &= \int_{-\infty}^{\infty} (w-u_\epsilon)(T,x) \, dx + \int_{-\infty}^{\infty} (u_\epsilon - u)(T,x) \, dx, \\ &= IIa + IIb, \end{aligned} \quad (4.3)$$

where recall that u_ϵ is the vanishing viscosity solution of (2.2).

Using the theory for the vanishing viscosity solution, we have

$$IIb = \mathbf{O}(\epsilon^{1/2}).$$

We can not estimate this term, since that requires the solution of the original problem, but we can make this term small by choosing ϵ small.

This leaves IIa to be estimated. The advantage gained by the decomposition (4.3) is that we have reduced the *a posteriori* analysis to solutions of problems that have well defined adjoint problems. We now consider the solution w of the modified equation as a perturbed solution of the vanishing viscosity problem (2.2). We use the solution η of the adjoint (2.3) for the vanishing viscosity problem. The analysis is exactly the same as for Theorem 3.1. We obtain

$$\int_{-\infty}^{\infty} (w - u_\epsilon)(T, x)\, dx = -\int_0^T \int_{-\infty}^{\infty} R_w \eta \, dxdt, \tag{4.4}$$

where the residual is

$$R_w = (c(h, k) - \epsilon) w_{xx}.$$

We summarize

THEOREM 4.1. *Let u denote the solution of the original problem, U denote the Lax-Friedrichs approximation, $\tilde{R}_U$ denote the residual of U in the modified equation, ϕ denote the solution of the adjoint for the modified equation, R_w the residual of the solution of the modified equation in the vanishing viscosity problem, η the solution of the adjoint for the vanishing viscosity problem, and $\epsilon > 0$ a small number. Then,*

$$\int_{-\infty}^{\infty} (U - u)(T, x)\, dx = \int_0^T \int_{\infty}^{\infty} \tilde{R}_U \phi \, dxdt + \int_0^T \int_{\infty}^{\infty} R_w \eta \, dxdt + \mathbf{O}(\epsilon^{1/2}). \tag{4.5}$$

Using (4.5) requires computing approximations of the adjoint solutions ϕ and η. The residual $\tilde{R}_U$ can be computed directly by substitution. The integrand in the second term

$$R_w = \left(\frac{h^2}{2k} \left(1 - \left(\frac{ak}{h} \right)^2 \right) - \epsilon \right) w_{xx} \eta$$

is small in regions where η and w_{xx} are small. Otherwise, we must make it small by choosing h and k so that

$$\frac{h^2}{2k} \left(1 - \left(\frac{ak}{h} \right)^2 \right) \approx \epsilon,$$

which effectively places a size restriction on the discretization. It would be interesting to pursue adaptive error control based on this criterion.

REMARK 4.1. *Extension of this analysis to the Lax-Wendroff scheme is an interesting problem. Because the modified equation for the Lax-Wendroff scheme involves a third order spatial derivative, we could use a Hermite spline with continuous first derivatives to define the function U in order to evaluate the residual in the weak error representation formula. The residual of U would now be*

$$R_w = \frac{h^2 a}{6} \left(\frac{a^2 k^2}{h^2} - 1 \right) w_{xxx} - \epsilon w_{xx}.$$

It is not clear that this expression can be made small!

This situation suggests the use of a blended scheme that becomes Lax-Wendroff in regions where the solution is smooth but Lax-Friedrichs in regions where the solution is nonsmooth. The analogous estimates for such a blended scheme might indicate how the blending should be carried out in an adaptive fashion as the solution progresses.

4.2. An *a posteriori* analysis of the time error in discontinuous Galerkin discretization. We next present an *a posteriori* error analysis for the numerical solution of the systems of ordinary differential equations that result after discretizing a system of conservation laws using the discontinuous Galerkin method in space. The discontinuous Galerkin method with an appropriate choice of flux function yields many of the standard finite difference approximations.

Following Cockburn [5], we consider the problem

$$\begin{cases} u_t + f(u)_x = 0, & 0 < x < 1,\, 0 < t < T, \\ u(0,t) = u(1,t), & 0 < t < T, \\ u(x,0) = u_0(x), & 0 < x < 1. \end{cases} \tag{4.6}$$

4.2.1. Discretization in space. We partition $(0,1)$ into $\{x_{j+1/2}\}_{j=0}^N$ and set $J = (x_{j-1/2}, x_{j+1/2})$, $h_j = x_{j+1/2} - x_{j-1/2}$ for $j = 1, \cdots, N$. For simplicity, we assume that $h_j = h$ for all j.

We compute a semidiscrete approximation $u_h(t)$ to $u(t)$ such that for each $0 < t < T$, u_h belongs to

$$V_h = \left\{ v \in L^1(0,1) : v|_{J_j} \in \mathcal{P}^0(J_j),\, j = 1, \cdots, N \right\},$$

where $P^0(J_j)$ denotes the constant polynomials on the interval.

The weak formulation of (4.6) over J_j reads

$$\begin{cases} \int_{J_j} \partial_t u(x,t) v(x)\, dx - \int_{J_j} f(u(x,t)) \partial_x v(x)\, dx \\ \qquad\qquad + f(u(x_{j+1/2},t)) v(x_{j+1/2}^-) - f(u(x_{j-1},t)) v(x_{j-1/2}^+) = 0, \\ \int_{J_j} u(x,0) v(x)\, dx = \int_{J_j} u_0(x) v(x)\, dx, \end{cases} \tag{4.7}$$

for $j = 1, \cdots, N$.

To formulate the finite element approximation, which is discontinuous across nodes, we replace the flux f by a numerical flux,

$$f(u(x_{j+1/2},t)) \to h(u(x_{j+1/2}^-,t), u(x_{j+1/2}^+,t)).$$

Since $u_h(x,t)$ is constant on each J_j, we write

$$u_j(t) = u_h(x,t),\, x \in J_j.$$

The semidiscrete discontinuous Galerkin finite element approximation satisfies

$$\begin{cases} \partial_t u_j(t) + \big(h(u_j(t), u_{j+1}(t)) - h(u_{j-1}(t), u_j(t)) \big)/h = 0, \\ u_j(0) = \int_{J_j} u_0(x)\, dx, \end{cases} \tag{4.8}$$

for $j = 1, \cdots, N$.

Various choices of the numerical flux lead to well known finite difference schemes. We consider the Lax-Friedrichs flux

$$h(a,b) = \frac{1}{2}(f(a) + f(b) - C(b-a))$$

where the classic Lax-Friedrichs scheme uses $C = 1$, but another choice is

$$C = \max_{\inf u_h \le s \le \sup u_h} |f'(s)|.$$

This yields the system

$$\begin{cases}\partial_t u_j(t) = -\frac{1}{2h}\big(f(u_{j+1}(t)) - f(u_{j-1}(t)) + \frac{C}{2}\big(u_{j+1} - u_{j-1}\big),\\ u_j(0) = \int_{J_j} u_0(x)\,dx,\end{cases} \tag{4.9}$$

for $j = 1, \cdots, N$. Imposing periodic boundary conditions, we can write this as

$$\begin{cases}\partial_t u_1(t) = -\frac{1}{2h}\big(f(u_2(t)) - f(u_N(t)) + \frac{C}{2}\big(u_2 - u_N\big),\\ \partial_t u_j(t) = -\frac{1}{2h}\big(f(u_{j+1}(t)) - f(u_{j-1}(t)) + \frac{C}{2}\big(u_{j+1} - u_{j-1}\big), \quad 2 \le j \le N-1,\\ \partial_t u_N(t) = -\frac{1}{2h}\big(f(u_1(t)) - f(u_{N-1}(t)) + \frac{C}{2}\big(u_1 - u_{N-1}\big),\\ u_j(0) = \int_{J_j} u_0(x)\,dx,\end{cases} \tag{4.10}$$

4.3. Discretization in time. We set

$$g(u) = \begin{pmatrix} -\frac{1}{2h}\big(f(u_2(t)) - f(u_N(t)) + \frac{C}{2}\big(u_2 - u_N\big) & \\ -\frac{1}{2h}\big(f(u_{j+1}(t)) - f(u_{j-1}(t)) + \frac{C}{2}\big(u_{j+1} - u_{j-1}\big) & j = 2, \cdots N, \\ -\frac{1}{2h}\big(f(u_1(t)) - f(u_{N-1}(t)) + \frac{C}{2}\big(u_1 - u_{N-1}\big) & \end{pmatrix}$$

so (4.10) becomes simply

$$u'(t) = g(u),\ 0 < t < T. \tag{4.11}$$

To discretize in time, we also use a discontinuous Galerkin method with piecewise constant approximations. We discretize $[0, T]$ by $\{t_i\}$ with $t_0 = 0$, $t_M = T$, $t_i - t_{i-1} = k$, and $I_i = (t_{i-1}, t_i]$ for all i. We set $U_j^0 = u_j(0)$ for $j = 1, \cdots, N$. For an implicit approximation for $i = 1, \cdots, M$, we compute U so that $U|_{I_i} \in \mathcal{P}^0(I_i)$ satisfies

$$\int_{I_i} (U_t - g(U)) \cdot v\,dt + \big(U_i - U_{i-1}\big) \cdot v_{i-1} = 0, \tag{4.12}$$

for all v with $v|_{I_i} \in \mathcal{P}^0(I_i)$. Note that $U_t \equiv 0$. We use an explicit approximation computed by applying the left-hand point rectangle rule to evaluate the integral

$$\int_{I_i} g(U) \cdot v\,dt \to g(U_{i-1})k \cdot v.$$

We end up with

$$U^i = U^{i-1} + kg(U^{i-1}). \tag{4.13}$$

This can be rewritten as the Lax-Friedrichs scheme,

$$U_j^{i+1} = U_j^i - \frac{k}{2h}\big(f(U_{j+1}^i) - f(U_{j-1}^i)\big) + \frac{Ck}{2}\big(U_{j+1}^i - U_{j-1}^i\big), \tag{4.14}$$

with suitable interpretation on the boundaries.

4.4. An *a posteriori* analysis of the time error. We analyze the error from discretization in time assuming that the space discretization is fixed.

Since the problem (4.10) is nonlinear, we linearize to form an adjoint problem.

We define

$$\bar{g}'(u,U) = \int_0^1 g'(sU + (1-s)u)\,ds,$$

so that

$$\bar{g}'(u,U)(U-u) = g(U) - g(u).$$

We define the adjoint problem

$$\begin{cases} -\phi'(t) - \bar{g}'(u,U)^\top \phi = 0, & T > t \geq 0, \\ \phi(T) = \psi. \end{cases} \tag{4.15}$$

This corresponds to the quantity of interest $u(T) \cdot \psi$. We set $e = U - u$.

Using the standard analysis for the discontinuous Galerkin method ([7]), we obtain the error representation

$$e(T) \cdot \psi = \sum_{i=1}^{M} \int_{I_i} (U' - g(U)) \cdot (\phi - \pi_k \phi)\,dt + \sum_{i=1}^{M} U^{i-1} \cdot (\phi - \pi_k \phi)|_{t=t_{i-1}}, \tag{4.16}$$

where π_k is any projection into the piecewise constant functions with respect to the discretization $\{t_i\}$. We choose the projection to interpolate ϕ at the nodes, which causes the second term to vanish. We obtain

$$e(T) \cdot \psi = \sum_{i=1}^{M} \int_{I_i} (U' - g(U)) \cdot (\phi - \phi(t_{i-1}))\,dt. \tag{4.17}$$

To use (4.17), we compute a numerical solution of (4.15), typically replacing

$$\bar{g}'(u,U) \to g'(U).$$

We solve this with a second order or higher method in order to be able to evaluate the projection expression.

We have to alter the representation (4.17) in order to treat the explicit method (4.13) used in practice. This becomes

$$\begin{aligned} e(T) \cdot \psi = \sum_{i=1}^{M} \int_{I_i} & (U' - g(U)) \cdot (\phi - \phi(t_{i-1}))\,dt \\ & + \sum_{i=1}^{M} \int_{I_i} (g(U) - g(U^{i-1}) \cdot (\phi - \phi(t_{i-1}))\,dt. \end{aligned} \tag{4.18}$$

The first expression on the right simplifies

$$\sum_{i=1}^{M} \int_{I_i} (U' - g(U)) \cdot (\phi - \phi(t_{i-1}))\,dt = -\sum_{i=1}^{M} g(U^i) \cdot \int_{I_i} (\phi - \phi(t_{i-1}))\,dt.$$

The second expression on the right

$$\sum_{i=1}^{M} \int_{I_i} (g(U) - g(U^{i-1}) \cdot (\phi - \phi(t_{i-1}))\, dt$$
$$= \sum_{i=1}^{M} (g(U^i) - g(U^{i-1}) \cdot \int_{I_i} (\phi - \phi(t_{i-1}))\, dt \quad (4.19)$$

is a quadrature error term.

4.4.1. A computational example. We discretize the problem

$$\begin{cases} u_t + uu_x = 0, & 0 < x < 1, 0 < t, \\ u(0,t) = u(1,t), & 0 < t, \\ u(x,0) = u_0(x), & 0 < x < 1, \end{cases} \quad (4.20)$$

in space using the dG/Lax-Friedrichs method with 50 space nodes, where

$$u_0(x) = \begin{cases} 0, & 0 < x < .4, \\ (x - .4)/.1, & .4 < x < .5, \\ (.6 - x)/.1, & .5 < x < .6, \\ 0, & .6 < x < 1. \end{cases}$$

We then use the estimate (4.18) to compute *a posteriori* estimates in the error of the average value.

We wish to understand the different sources of error, so we compare the results from using both the implicit and explicit Euler methods for the time integration. The implicit Euler error representation does not have the quadrature error term (4.19).

We show the implicit Euler results in Fig. 4.1.

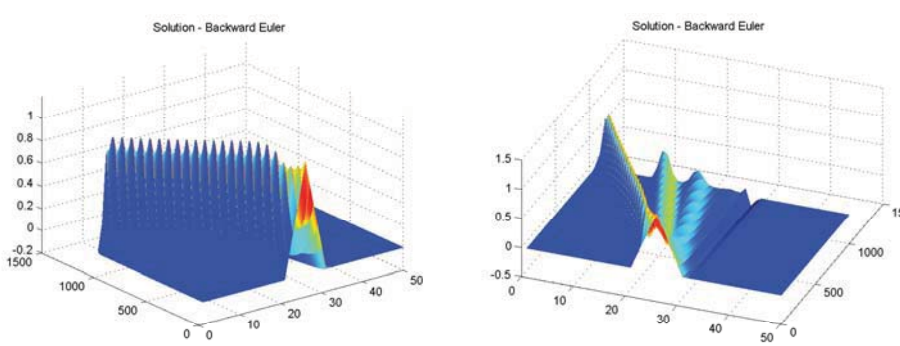

Fig. 4.1: A solution of the semidiscrete Burgers equation computed using the dG method in space and implicit Euler in time. The plot on the right is rotated.

We show the results using explicit Euler for time integration, yielding the common scheme (4.14), in Fig. 4.2.

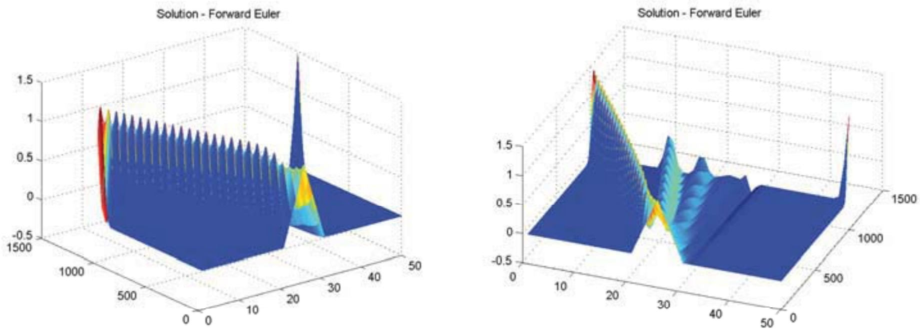

Fig. 4.2: A solution of the semidiscrete Burgers equation computed using the dG method in space and explicit Euler in time. The plot on the right is rotated.

We plot the element contributions in (4.16), i.e.

$$\int_{I_i} (U' - g(U)) \cdot (\phi - \pi_k \phi)\, dt + U^{i-1} \cdot (\phi - \pi_k \phi)|_{t=t_{i-1}},$$

for each component of the solution in Fig. 4.3. The explicit Euler method clearly exhibits some mild instability as the element contributions increase in time, whereas the implicit Euler contributions remain bounded.

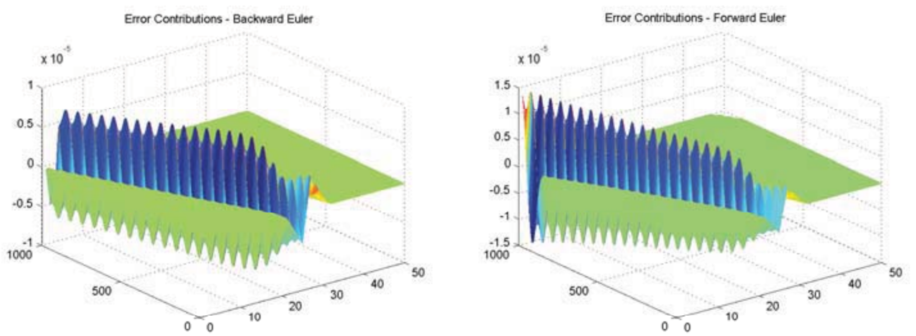

Fig. 4.3: We plot the element error contributions for the implicit and explicit Euler methods. Note the gradual increase in the error contributions for the explicit Euler scheme as time increases (back towards the upper left). This suggests that the explicit Euler exhibits some mild instability.

Next we plot the element contributions

$$(g(U^i) - g(U^{i-1}) \cdot \int_{I_i} (\phi - \phi(t_{i-1}))\, dt$$

for the quadrature error component. This has a very interesting pattern in that the quadrature error increases as time passes in all the variables uniformly, see Fig. 4.4. In fact, the quadrature error comes to dominate the entire error!

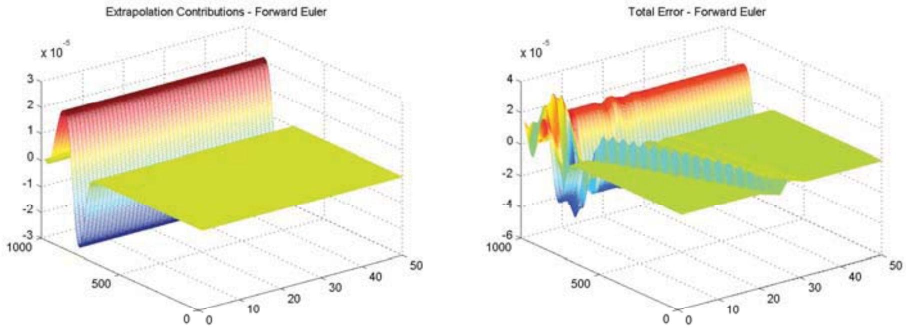

Fig. 4.4: Left: Quadrature error contributions for the explicit Euler solution. Right: Total error estimate for the explicit Euler solution.

5. An *a posteriori* analysis for the MAC scheme for the Navier-Stokes problem. The Navier-Stokes equations describe the flow of fluids. The system of equations comes about through expressions of the three conservation laws: mass, momentum, and energy and is written as,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0, \tag{5.1}$$

$$\rho \frac{\partial \mathbf{V}}{\partial t} + \rho(\mathbf{V} \cdot \nabla)\mathbf{V} = \rho \mathbf{g} + \nabla \cdot \tau'_{ij} - \nabla p, \tag{5.2}$$

$$\rho \frac{\partial h}{\partial t} + \rho(\mathbf{V} \cdot \nabla)h = \frac{\partial p}{\partial t} + \rho(\mathbf{V} \cdot \nabla)p + \nabla \cdot (k\nabla T) + \tau'_{ij}\frac{\partial u_i}{\partial x_j}. \tag{5.3}$$

Here ρ is density, $\mathbf{V} = (u_1, u_2, u_3)$ is velocity, p is pressure, $\mathbf{g}$ are gravitational forces, k is the thermal conductivity, and h is enthalpy expressed as, $h = e + \frac{p}{\rho}$ where e is internal energy. For a linear, Newtonian fluid, the viscous stresses are expressed as,

$$\tau'_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \delta_{ij}\lambda \nabla \cdot \mathbf{V}, \tag{5.4}$$

where μ is the coefficient of viscosity, and λ is the coefficient of bulk viscosity.

5.1. The stationary problem and discretization. We describe the discretization and analysis for a stationary version of the incompressible Navier-Stokes equation in velocity-pressure formulation on domain $\Omega \subset \mathbb{R}^2$, i.e.

$$-\nu\Delta\mathbf{u} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} + \nabla p = \boldsymbol{F}, \quad \text{in } \Omega \tag{5.5a}$$

$$-\nabla \cdot \mathbf{u} = \mathbf{0} \quad \text{in } \Omega \tag{5.5b}$$

$$\mathbf{u} = \mathbf{0}, \quad \text{on } \partial\Omega. \tag{5.5c}$$

Here, $\nu > 0$ is the kinematic viscosity and $\mathbf{u} = (u^x, u^y)$ and p are the velocity and pressure unknowns. $\boldsymbol{F} = (F^x, F^y)$ is the given volume force.

Extending the analysis to a discretization of the full time-dependent version of the problem is relatively straightforward.

5.1.1. A mixed finite element scheme. Let $H^n(\Omega)$ and $H_0^1(\Omega)$ be the standard Sobolev spaces equipped with the norm $\|\cdot\|_{n,\Omega}$ and let

$$\mathbf{V} = H_0^1(\Omega) \times H_0^1(\Omega),$$
$$M = \left\{ q \in L^2(\Omega) \text{ and } \int_\Omega q\,\mathrm{d}x = 0 \right\}.$$

Then the weak formulation for (5.5) is, find $(\mathbf{u}, p) \in (\mathbf{V}, M)$ such that

$$a(\mathbf{u},\mathbf{v}) + b(\mathbf{v},p) + c(\mathbf{u},\mathbf{v}) = (\boldsymbol{F},\mathbf{v}), \quad \forall\, \mathbf{v} \in \mathbf{V}, \tag{5.6a}$$
$$b(\mathbf{u},q) = 0, \quad \forall\, q \in M, \tag{5.6b}$$

where

$$a(\mathbf{u},\mathbf{v}) = \nu \int_\Omega \nabla\mathbf{u} : \nabla\mathbf{v}\,\mathrm{d}x,$$
$$b(\mathbf{u},q) = -\int_\Omega q\nabla\cdot\mathbf{v}\,\mathrm{d}x,$$
$$c(\mathbf{u},\mathbf{v}) = \int_\Omega (\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\mathbf{v}\,\mathrm{d}x,$$
$$(\boldsymbol{F},\mathbf{v}) = \int_\Omega \boldsymbol{F}\cdot\mathbf{v}\,\mathrm{d}x.$$

For simplicity, we take Ω to be a unite square $[0,1]\times[0,1]$ and we partition $[0,1]$ in x- and y- direction as following:

$$0 = x_0 < x_1 < \cdots < x_k = 1; \qquad 0 = y_0 < y_1 < \cdots < y_\ell = 1.$$

The corresponding quadrangulation is denoted by $\mathcal{T}_h$. We also denote the middle points with indices of half integers: $x_{i+1/2} = (x_{i+1} - x_i)/2$, $y_{j+1/2} = (y_{j+1} - y_j)/2$. Interval distances are $\Delta x_{i+1/2} = x_{i+1} - x_i$, $\Delta y_{j+1/2} = y_{j+1} - y_j$ for $i = 0,1,\cdots,k-1$, $j = 0,1,\cdots,\ell-1$, and $\Delta x_i = x_{i+1/2} - x_{i-1/2}$, $\Delta y_j = y_{j+1/2} - y_{j-1/2}$ for $i = 1,\cdots,k-1$, $j = 1,\cdots,\ell-1$. We connect all the midpoints of the vertical sides of $\mathcal{T}_h$ by straight line segments. The corresponding quadrangulation is denoted by $\mathcal{T}_h^1$. Similarly, if we connect all the midpoints of the horizontal sides of $\mathcal{T}_h$, then we obtain the third quadrangulation which is denoted by $\mathcal{T}_h^2$. We denote $h = \max(\Delta x_{i+1/2}, i = 0,\cdots,k-1; \Delta y_{j+1/2}, j = 0,\cdots,\ell-1)$.

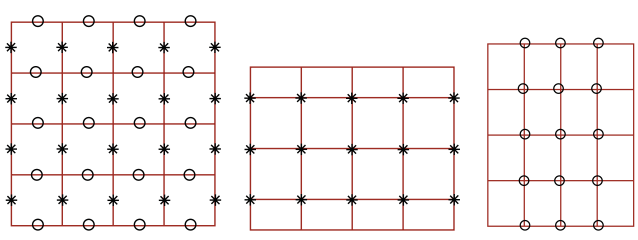

Fig. 5.1: Quadrangulations: (a) $\mathcal{T}_h$, (b) $\mathcal{T}_h^1$, (c) $\mathcal{T}_h^2$.

Note that different discretizations and approximation spaces are assigned to the three primitive variables p, u^x and u^y. Specifically, p is approximated by piecewise constant on each cell $[x_{i-1}, x_i] \times [y_{j-1}, y_j]$ with degree of freedom located at the center. That is, the approximate solution P belongs to

$$M_h = \left\{ q_h : q_h|_K = \text{ constant } \forall K \in \mathcal{T}_h \text{ and } \int_\Omega q_h \, \mathrm{d}x = 0 \right\}.$$

As for velocity approximation U^x and U^y, we have

$$U^x \in S_h^1 = \left\{ v_h \in C^0(\bar{\Omega}) : v_h|_K \in Q_1(K), \forall K \in \mathcal{T}_h^1, \text{ and } v_h|_{\partial\Omega} = 0 \right\},$$
$$U^y \in S_h^2 = \left\{ v_h \in C^0(\bar{\Omega}) : v_h|_K \in Q_1(K), \forall K \in \mathcal{T}_h^2, \text{ and } v_h|_{\partial\Omega} = 0 \right\}.$$

Here, Q_1 denotes the bilinear space. Let

$$\mathbf{V}_h = S_h^1 \times S_h^2 \subset \mathbf{V}.$$

Then the discrete mixed finite element scheme becomes, find $(\mathbf{U}, P) \in \mathbf{V}_h \times M_h$ such that

$$a(\mathbf{U}, \mathbf{v}) + b(\mathbf{v}, P) + c(\mathbf{U}, \mathbf{v}) = (\boldsymbol{F}, \mathbf{v}), \quad \forall \, \mathbf{v} \in \mathbf{V}_h, \tag{5.7a}$$
$$b(\mathbf{U}, q) = 0, \quad \forall \, q \in M_h. \tag{5.7b}$$

For the quadrangulation $\mathcal{T}_h$, we divide the edges of all squares into two sets. The set containing all vertical edges is denoted by L_V, and the set containing all horizontal edges is denoted by L_H. We are then able to define an operator $I_h : \mathbf{V} \mapsto \mathbf{V}_h$ by

$$I_h \mathbf{u} = (I_h^1 u^x, I_h^2 u^y) \in S_h^1 \times S_h^2 \;\text{ satisfying}$$
$$\int_l I_h^1 u^x \mathrm{d}s = \int_l u^x \mathrm{d}s \quad \forall \, l \in L_V, \tag{5.8}$$
$$\int_l I_h^2 u^y \mathrm{d}s = \int_l u^y \mathrm{d}s \quad \forall \, l \in L_H. \tag{5.9}$$

As proven in [9], the following properties of this operator are observed :

(i) for all $\mathbf{u} \in \mathbf{V}$,

$$\int_\Omega q_h \, \mathrm{div}(\mathbf{u} - I_h \mathbf{u}) \, \mathrm{d}x = 0 \quad \forall q_h \in M_h.$$

(ii) there exists constant C_1 independent of mesh size, such that

$$\|\mathbf{u} - I_h \mathbf{u}\|_{1,\Omega} \le C_1 h |\mathbf{u}|_{2,\Omega}, \quad \forall \mathbf{u} \in \mathbf{V}.$$

(iii) there is a constant C_2 independent of mesh size, such that

$$\|I_h \mathbf{u}\|_{1,\Omega} \le C_2 \|\mathbf{u}\|_{1,\Omega}, \quad \forall \mathbf{u} \in \mathbf{V}.$$

5.1.2. The MAC finite volume scheme. We now derive a mark and cell (MAC) finite volume scheme for (5.5). First, integrate the x- and y-component of the momentum equation and the continuity equation on different finite volumes; Next, we approximate each term within proper approximation spaces. The following notations are used in the scheme

$$\hat{\hat{\eta}}_{i,j-1/2} = \frac{1}{4}\left(\eta_{i-1/2,j-1} + \eta_{i+1/2,j-1} + \eta_{i-1/2,j} + \eta_{i+1/2,j}\right),$$

$$\delta_x \eta_{i+1/2,j-1/2} = \frac{\eta_{i+1,j-1/2} - \eta_{i,j-1/2}}{\Delta x_{i+1/2}} \qquad \delta_y \eta_{i,j} = \frac{\eta_{i,j+1/2} - \eta_{i,j-1/2}}{\Delta y_j} \qquad \forall \eta \in S_h^1,$$

and

$$\hat{\hat{\xi}}_{i-1/2,j} = \frac{1}{4}\left(\xi_{i-1,j-1/2} + \xi_{i,j-1/2} + \xi_{i-1,j+1/2} + \xi_{i,j+1/2}\right),$$

$$\delta_x \xi_{i,j} = \frac{\xi_{i+1/2,j} - \xi_{i-1/2,j}}{\Delta x_i} \qquad \delta_y \xi_{i-1/2,j+1/2} = \frac{\xi_{i-1/2,j+1} - \xi_{i-1/2,j-1}}{\Delta y_j} \qquad \forall \xi \in S_h^2.$$

The x-component of momentum. On $K = [x_{i-1/2}, x_{i+1/2}] \times [y_{j-1}, y_j] \in \mathcal{T}_h^1$, $i = 1, \cdots, k-1, j = 1, \cdots, \ell$, we have

$$\begin{aligned}
&-\nu \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1}}^{y_j} \frac{\partial^2 U^x}{\partial x^2} + \frac{\partial^x U^x}{\partial y^2}\, \mathrm{d}y \mathrm{d}x \\
&\quad = -\nu \int_{y_{j-1}}^{y_j} \frac{\partial U^x}{\partial x}|_{x_{i+1/2}} - \frac{\partial U^x}{\partial x}|_{x_{i-1/2}}\, \mathrm{d}y - \nu \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial U^x}{\partial y}|_{y_j} - \frac{\partial U^x}{\partial y}|_{y_{j-1}}\, \mathrm{d}x \\
&\quad = -\nu \Delta y_{j-1/2} \delta_x U^x_{i+1/2,j-1/2} + \nu \Delta y_{j-1/2} \delta_x U^x_{i-1/2,j-1/2} \qquad (5.10) \\
&\qquad - \nu \Delta x_i \delta_y U^x_{i,j} + \nu \Delta x_i \delta_y U^x_{i,j-1}.
\end{aligned}$$

In the last step, all the gradients are approximated by cell-centered finite difference. On the boundary elements, we enforce the boundary condition and get

For the nonlinear diffusion term, we have

$$\begin{aligned}
&\int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1}}^{y_j} (\mathbf{U} \cdot \nabla)\, U^x\, \mathrm{d}y \mathrm{d}x = \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1}}^{y_j} U^y \frac{\partial U^x}{\partial y} + U^x \frac{\partial U^x}{\partial x}\, \mathrm{d}y \mathrm{d}x \\
&= \hat{\hat{U}}^y{}_{i,j-1/2} \int_{x_{i-1/2}}^{x_{i+1/2}} U^x|_{y_j} - U^x|_{y_{j-1}}\, \mathrm{d}x + U^x_{i,j-1/2} \int_{y_{j-1}}^{y_j} U^x|_{x_{i+1/2}} - U^x|_{x_{i-1/2}}\, \mathrm{d}y \\
&= \hat{\hat{U}}^y{}_{i,j-1/2} \Delta x_i \frac{U^x_{i,j+1/2} - U^x_{i,j-3/2}}{2} + U^x_{i,j-1/2} \Delta y_{j-1/2} \frac{U^x_{i+1,j-1/2} - U^x_{i-1,j-1/2}}{2}. \qquad (5.11)
\end{aligned}$$

Here, in the second equation, U^y is approximated by the average of the four neighbors and U^x is approximated by the center value on the cell. While, in the third equation, U^x and U^y are approximated by the average of their two neighbors. For the pressure gradient term, we have

$$\begin{aligned}
\int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1}}^{y_j} \frac{\partial P}{\partial x}\, \mathrm{d}y \mathrm{d}x &= \int_{y_{j-1}}^{y_j} P|_{x_{i+1/2}} - P|_{x_{i-1/2}}\, \mathrm{d}y \\
&= \left(P_{i+1/2,j-1/2} - P_{i-1/2,j-1/2}\right) \Delta y_{j-1/2}. \qquad (5.12)
\end{aligned}$$

Finally, for the source term, we have

$$\int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j-1}}^{y_j} F^x \, \mathrm{d}y \mathrm{d}x = F^x_{i,j-1/2} \Delta x_i \Delta y_{j-1/2}. \tag{5.13}$$

The y-component of momentum. The y-component of the momentum equation is integrated on $[x_{i-1}, x_i] \times [y_{j-1/2}, y_{j+1/2}] \in \mathcal{T}_h^2, i = 1, \cdots, k, j = 1, \cdots, \ell - 1$. Each integral can be handled in a similar way as for x-component. So we have

$$\begin{aligned} -\nu \int_{x_{i-1}}^{x_i} \int_{y_{j-1/2}}^{y_{j+1/2}} \frac{\partial^2 U^y}{\partial x^2} + \frac{\partial^2 U^y}{\partial y^2} \, \mathrm{d}y \mathrm{d}x &= -\nu \Delta y_j \delta_x U^y_{i,j} + \nu \Delta y_j \delta_x U^y_{i-1,j} \\ &- \nu \Delta x_{i-1/2} \delta_y U^y_{i-1/2,j+1/2} + \nu \Delta x_{i-1/2} \delta_y U^y_{i-1/2,j-1/2}. \end{aligned} \tag{5.14}$$

$$\begin{aligned} \int_{x_{i-1}}^{x_i} \int_{y_{j-1/2}}^{y_{j+1/2}} (\mathbf{U} \cdot \nabla) U^y \, \mathrm{d}y \mathrm{d}x &= \hat{\hat{U}}^x{}_{i-1/2,j} \Delta y_j \frac{U^y_{i+1/2,j} - U^y_{i-3/2,j}}{2} \\ &+ U^y_{i-1/2,j} \Delta x_{i-1/2} \frac{U^y_{i-1/2,j+1} - U^y_{i-1/2,j-1}}{2}. \end{aligned} \tag{5.15}$$

$$\begin{aligned} \int_{x_{i-1}}^{x_i} \int_{y_{j-1/2}}^{y_{j+1/2}} \frac{\partial P}{\partial y} \, \mathrm{d}y \mathrm{d}x &= \int_{x_{i-1}}^{x_i} P|_{y_{j+1/2}} - P|_{y_{j-1/2}} \, \mathrm{d}x \\ &= \left(P_{i-1/2,j+1/2} - P_{i-1/2,j-1/2} \right) \Delta x_{i-1/2}. \end{aligned} \tag{5.16}$$

$$\int_{x_{i-1}}^{x_i} \int_{y_{j-1/2}}^{y_{j+1/2}} F^y \, \mathrm{d}y \mathrm{d}x = F^y_{i-1/2,j} \Delta x_{i-1/2} \Delta y_j. \tag{5.17}$$

The continuity equation. For the continuity equation, we integrate over $K = [x_{i-1}, x_i] \times [y_{j-1}, y_j] \in \mathcal{T}_h, i = 1, \cdots, k, \; j = 1, \cdots, \ell$,

$$\int_{x_{i-1}}^{x_i} \int_{y_{j-1}}^{y_j} -\nabla \cdot \mathbf{U} \, \mathrm{d}y \mathrm{d}x = -\int_{x_{i-1}}^{x_i} U^y|_{y_j} - U^y|_{y_{j-1}} \, \mathrm{d}x - \int_{y_{j-1}}^{y_j} U^x|_{x_i} - U^x|_{x_{i-1}} \, \mathrm{d}y.$$

With U^x and U^y approximated by the average of the corresponding neighbors, we obtain

$$-\Delta x_{i-1/2} \Delta y_{j-1/2} \left\{ \delta_x U^x_{i-1/2,j-1/2} + \delta_y U^y_{i-1/2,j-1/2} \right\} = 0. \tag{5.18}$$

We now collect all the terms and get the following MAC scheme:

$$
\begin{aligned}
&-\nu\Delta y_{j-1/2}\delta_x U^x_{i+1/2,j-1/2} + \nu\Delta y_{j-1/2}\delta_x U^x_{i-1/2,j-1/2} - \nu\Delta x_i \delta_y U^x_{i,j} + \nu\Delta x_i\delta_y U^x_{i,j-1}\\
&+ \hat{\hat{U}}^y{}_{i,j-1/2}\Delta x_i \frac{U^x_{i,j+1/2} - U^x_{i,j-3/2}}{2} + U^x_{i,j-1/2}\Delta y_{j-1/2}\frac{U^x_{i+1,j-1/2} - U^x_{i-1,j-1/2}}{2}\\
&+ \left(P_{i+1/2,j-1/2} - P_{i-1/2,j-1/2}\right)\Delta y_{j-1/2} = F^x_{i,j-1/2}\Delta x_i \Delta y_{j-1/2}
\end{aligned}
\tag{5.19}
$$

$$
\begin{aligned}
&-\nu\Delta y_j \delta_x U^y_{i,j} + \nu\Delta y_j\delta_x U^y_{i-1,j} - \nu\Delta x_{i-1/2}\delta_y U^y_{i-1/2,j+1/2} + \nu\Delta x_{i-1/2}\delta_y U^y_{i-1/2,j-1/2}\\
&+ \hat{\hat{U}}^x{}_{i-1/2,j}\Delta y_j \frac{U^y_{i+1/2,j} - U^y_{i-3/2,j}}{2} + U^y_{i-1/2,j}\Delta x_{i-1/2}\frac{U^y_{i-1/2,j+1} - U^y_{i-1/2,j-1}}{2}\\
&+ \left(P_{i-1/2,j+1/2} - P_{i-1/2,j-1/2}\right)\Delta x_{i-1/2} = F^y_{i-1/2,j}\Delta x_{i-1/2}\Delta y_j
\end{aligned}
\tag{5.20}
$$

$$
-\Delta x_{i-1/2}\Delta y_{j-1/2}\left(\delta_x U^x_{i-1/2,j-1/2} + \delta_y U^y_{i-1/2,j-1/2}\right) = 0. \tag{5.21}
$$

5.2. An *a posteriori* error analysis. In order to rewrite (5.19), (5.20) and (5.21) into the framework of mixed finite element scheme, we first define the following interpolating operators as in [9]:

$$
\begin{aligned}
\mathcal{Q}^1_h:\quad & C^0(\bar{K}_1) \longrightarrow Q_1(K_1),\ \text{such that}\\
& (\mathcal{Q}^1_h\phi)(a_i) := \phi(a_i), i = 1,2,3,4,
\end{aligned}
\tag{5.22}
$$

where a_i, $i = 1,2,3,4$, are the four nodes of $K_1 \in \mathcal{T}^1_h$,

$$
\begin{aligned}
\mathcal{Q}^2_h:\quad & C^0(\bar{K}_2) \longrightarrow Q_1(K_2),\ \text{such that}\\
& (\mathcal{Q}^2_h\phi)(b_i) := \phi(b_i), i = 1,2,3,4,
\end{aligned}
\tag{5.23}
$$

where b_i, $i = 1,2,3,4$, are the four nodes of $K_2 \in \mathcal{T}^2_h$, and

$$
\begin{aligned}
\mathcal{Q}_h:\quad & C^0(\bar{K}) \longrightarrow Q_0(K),\ \text{such that}\\
& (\mathcal{Q}_h\phi)(c) := \phi(c),
\end{aligned}
\tag{5.24}
$$

where c is the center of $K_1 \in \mathcal{T}^1_h$. We then introduce the bilinear forms

$$
a_h(\mathbf{U},\mathbf{v}) = \nu\left\{\sum_{K_1\in\mathcal{T}^1_h}\int_{K_1}\mathcal{Q}^1_h(\nabla U^x\cdot\nabla v^x)\mathrm{d}x + \sum_{K_2\in\mathcal{T}^2_h}\int_{K_2}\mathcal{Q}^2_h(\nabla U^y\cdot\nabla v^y)\mathrm{d}x\right\},\qquad \forall\ \mathbf{U},\mathbf{v}\in\mathbf{V}_h,
$$

$$
b_h(\mathbf{U},q_h) = -\sum_{K\in\mathcal{T}_h}\int_K q_h\mathcal{Q}_h(\nabla\cdot\mathbf{U})\mathrm{d}x,\quad \forall\ \mathbf{U}\in\mathbf{V}_h, q_h\in M_h,
$$

and

$$c_h(\mathbf{U},\mathbf{v}) = \left(U^x \frac{\partial U^x}{\partial x}, v^x\right)_{M_c D_c M_c} + \left(U^y \frac{\partial U^x}{\partial y}, v^x\right)_{M_n D_c M_c} + \left(U^x \frac{\partial U^y}{\partial x}, v^y\right)_{M_n D_c M_c} + \left(U^y \frac{\partial U^y}{\partial y}, v^y\right)_{M_c D_c M_c}, \quad \forall\ \mathbf{U},\mathbf{v} \in \mathbf{V}_h,$$

where the subscripts M_c denotes midpoint approximations, M_n denotes the average of values on four vertex of any cell and D_c denotes centered finite difference. For the discretized source term, we define

$$\boldsymbol{F}_h(\mathbf{v}) = \sum_{K\in\mathcal{T}_h} \int_K \mathcal{Q}_h(\boldsymbol{F}\cdot\mathbf{v})\,\mathrm{d}x.$$

With suitably chosen test functions, the MAC scheme can be obtained in an equivalent form as

$$a_h(\mathbf{U},\mathbf{v}) + b_h(\mathbf{v},P) + c_h(\mathbf{U},\mathbf{v}) = \boldsymbol{F}_h(\mathbf{v}), \quad \forall \mathbf{v} \in \mathbf{V}_h, \tag{5.25a}$$

$$b_h(\mathbf{U},w) = 0, \quad \forall w \in M_h. \tag{5.25b}$$

Subtracting (5.25a) and (5.25b) from (5.7a) and (5.7b) respectively and denote $e_{\mathbf{u}} = \mathbf{u} - \mathbf{U}, e_p = p - P$, we obtain

$$\begin{aligned} \nu\left(\nabla e_{\mathbf{u}}, \nabla\mathbf{v}\right) - \left(e_p, \nabla\cdot\mathbf{v}\right) + \left\{\left(\left(\nabla\tilde{\mathbf{u}}\right)^\top \mathbf{v}, e_{\mathbf{u}}\right) - \left(\left(\nabla\cdot\tilde{\mathbf{u}}\right)e_{\mathbf{u}}, \mathbf{v}\right) - \left(\left(\tilde{\mathbf{u}}\cdot\nabla\right)\mathbf{v}, e_{\mathbf{u}}\right)\right\} \\ = \mathrm{QE1}(\mathbf{v}) + \mathrm{QE2}(P,\mathbf{v}) + \mathrm{QE3}(\mathbf{v}) + \mathrm{QE4}(\mathbf{v}), \quad \forall\ \mathbf{v} \in \mathbf{V}_h, \end{aligned} \tag{5.26}$$

$$-\left(\nabla\cdot e_{\mathbf{u}}, w\right) = \mathrm{QE2}(w,\mathbf{U}), \quad \forall\ w \in M_h, \tag{5.27}$$

where $\mathrm{QE1} - \mathrm{QE4}$ are quadratures errors defined as

$$\mathrm{QE1}(\mathbf{v}) = \nu\left\{\sum_{K_1\in\mathcal{T}_h^1} \int_{K_1} (\mathcal{Q}_h^1 - \mathbb{I})(\nabla U^x\cdot\nabla\mathbf{v}^x)\,\mathrm{d}x\mathrm{d}y + \sum_{K_2\in\mathcal{T}_h^2} \int_{K_2} (\mathcal{Q}_h^2 - \mathbb{I})(\nabla U^y\cdot\nabla\mathbf{v}^y)\,\mathrm{d}x\mathrm{d}y\right\}, \tag{5.28}$$

$$\mathrm{QE2}(q_h,\mathbf{v}) = -\sum_{K\in\mathcal{T}_h} \int_K q_h(\mathcal{Q}_h - \mathbb{I})\nabla\cdot\mathbf{v}\,\mathrm{d}x\mathrm{d}y, \tag{5.29}$$

$$\begin{aligned}
\mathrm{QE3}(\mathbf{v}) = & \left(U^x\frac{\partial U^x}{\partial x}, v^x\right) - \left(U^x\frac{\partial U^x}{\partial x}, v^x\right)_{M_cD_cM_c} \\
& + \left(U^y\frac{\partial U^x}{\partial y}, v^x\right) - \left(U^y\frac{\partial U^x}{\partial y}, v^x\right)_{M_nD_cM_c} \\
& + \left(U^x\frac{\partial U^y}{\partial x}, v^y\right) - \left(U^x\frac{\partial U^y}{\partial x}, v^y\right)_{M_nD_cM_c} \\
& + \left(U^y\frac{\partial U^y}{\partial y}, v^y\right) - \left(U^y\frac{\partial U^y}{\partial y}, v^y\right)_{M_cD_cM_c}, \qquad (5.30)
\end{aligned}$$

$$\mathrm{QE4}(\mathbf{v}) = \sum_{K\in\mathcal{T}_h}\int_K (\mathbb{I}-\mathcal{Q}_h)(\boldsymbol{F}\cdot\mathbf{v})\,\mathrm{d}x. \qquad (5.31)$$

Here, $\mathbb{I}$ denotes the identity operator. The three terms in the bracket of (5.26) are obtained by linearizing the nonlinear term $(\mathbf{u}\cdot\nabla)\mathbf{u}-(\mathbf{U}\cdot\nabla)\mathbf{U}$ around $\tilde{\mathbf{u}}=\frac{1}{2}(\mathbf{u}+\mathbf{U})$.

The adjoint problem of (5.7) is

$$\begin{aligned}
-\nu\Delta\boldsymbol{\phi}+(\nabla\tilde{\mathbf{u}})^\top\boldsymbol{\phi}-(\nabla\cdot\tilde{\mathbf{u}})\,\boldsymbol{\phi}-\tilde{\mathbf{u}}\cdot\nabla\boldsymbol{\phi}+\nabla z \;&=\; \boldsymbol{\psi}_{\mathbf{u}}, \quad \text{in } \Omega, && (5.32a)\\
-\nabla\cdot\boldsymbol{\phi} \;&=\; \psi_p, \quad \text{in } \Omega, && (5.32b)\\
\boldsymbol{\phi} \;&=\; \mathbf{0}, \quad \text{on } \partial\Omega. && (5.32c)
\end{aligned}$$

If we multiply $\boldsymbol{\phi}_{\mathbf{u}}$ and ψ_p to $e_{\mathbf{u}}$ and e_p respectively, integrate over Ω and add them up, we obtain

$$\begin{aligned}
&(e_{\mathbf{u}},\boldsymbol{\psi}_{\mathbf{u}})+(e_p,\psi_p)\\
=&\big(e_{\mathbf{u}},-\nu\Delta\boldsymbol{\phi}+(\nabla\tilde{\mathbf{u}})^\top\boldsymbol{\phi}-(\nabla\cdot\tilde{\mathbf{u}})\boldsymbol{\phi}-(\tilde{\mathbf{u}}\cdot\nabla)\boldsymbol{\phi}-(\nabla\cdot e_{\mathbf{u}},z)-(e_p,\nabla\cdot\boldsymbol{\phi})\big)\\
=&(\nu\nabla\boldsymbol{\phi},\nabla e_{\mathbf{u}})+\big(e_{\mathbf{u}},(\nabla\tilde{\mathbf{u}})^\top\boldsymbol{\phi}\big)-(e_{\mathbf{u}},(\nabla\cdot\tilde{\mathbf{u}})\boldsymbol{\phi})-(e_{\mathbf{u}},(\tilde{\mathbf{u}}\cdot\nabla)\boldsymbol{\phi})-(\nabla\cdot e_{\mathbf{u}},z)-(e_p,\nabla\cdot\boldsymbol{\phi})\\
=&(\nu\nabla\boldsymbol{\phi},\nabla e_{\mathbf{u}})+\big((\nabla\tilde{\mathbf{u}})^\top\boldsymbol{\phi},e_{\mathbf{u}}\big)-((\nabla\cdot\tilde{\mathbf{u}})e_{\mathbf{u}},\boldsymbol{\phi})-((\tilde{\mathbf{u}}\cdot\nabla)\boldsymbol{\phi},e_{\mathbf{u}})-(e_p,\nabla\cdot\boldsymbol{\phi})-(\nabla\cdot e_{\mathbf{u}},z)\\
=&(\nu\nabla(\boldsymbol{\phi}-I_h\boldsymbol{\phi}),\nabla e_{\mathbf{u}})+\big((\nabla\tilde{\mathbf{u}})^\top(\boldsymbol{\phi}-I_h\boldsymbol{\phi}),e_{\mathbf{u}}\big)-((\nabla\cdot\tilde{\mathbf{u}})e_{\mathbf{u}},\boldsymbol{\phi}-I_h\boldsymbol{\phi})\\
&-((\tilde{\mathbf{u}}\cdot\nabla)(\boldsymbol{\phi}-I_h\boldsymbol{\phi}),e_{\mathbf{u}})-(e_p,\nabla\cdot(\boldsymbol{\phi}-I_h\boldsymbol{\phi}))-(\nabla\cdot e_{\mathbf{u}},z-\mathbb{P}_hz)\\
&+(\nu\nabla I_h\boldsymbol{\phi},\nabla e_{\mathbf{u}})+\big((\nabla\tilde{\mathbf{u}})^\top I_h\boldsymbol{\phi},e_{\mathbf{u}}\big)-((\nabla\cdot\tilde{\mathbf{u}})e_{\mathbf{u}},I_h\boldsymbol{\phi})\\
&-((\tilde{\mathbf{u}}\cdot\nabla)I_h\boldsymbol{\phi},e_{\mathbf{u}})-(e_p,\nabla\cdot I_h\boldsymbol{\phi})-(\nabla\cdot e_{\mathbf{u}},\mathbb{P}_hz)\\
=&\{(\nu\nabla(\boldsymbol{\phi}-I_h\boldsymbol{\phi}),\nabla\mathbf{u})+((\mathbf{u}\cdot\nabla)\mathbf{u},\boldsymbol{\phi}-I_h\boldsymbol{\phi})-(p,\nabla\cdot(\boldsymbol{\phi}-I_h\boldsymbol{\phi}))\}+(\nabla\cdot\mathbf{U},z-\mathbb{P}_hz)\\
&-(\nu\nabla(\boldsymbol{\phi}-I_h\boldsymbol{\phi}),\nabla\mathbf{U})-((\mathbf{U}\cdot\nabla)\mathbf{U},\boldsymbol{\phi}-I_h\boldsymbol{\phi})+(P,\nabla\cdot(\boldsymbol{\phi}-I_h\boldsymbol{\phi}))-(\nabla\cdot\mathbf{u},z-\mathbb{P}_hz)\\
&+\{\mathrm{QE1}(I_h\boldsymbol{\phi}))+\mathrm{QE2}(P,I_h\boldsymbol{\phi})+\mathrm{QE3}(I_h\boldsymbol{\phi})++\mathrm{QE4}(I_h\boldsymbol{\phi})+\mathrm{QE2}(\mathbb{P}_hz,\mathbf{U})\}\\
=&\mathbb{T}_r+\{\mathrm{QE1}(I_h\boldsymbol{\phi})+\mathrm{QE2}(P,I_h\boldsymbol{\phi})+\mathrm{QE3}(I_h\boldsymbol{\phi})++\mathrm{QE4}(I_h\boldsymbol{\phi})+\mathrm{QE2}(\mathbb{P}_hz,\mathbf{U})\},
\end{aligned}$$

where

$$\begin{aligned}
\mathbb{T}_r=&-(\nu\nabla(\boldsymbol{\phi}-I_h\boldsymbol{\phi}),\nabla\mathbf{U})-((\mathbf{U}\cdot\nabla)\mathbf{U},\boldsymbol{\phi}-I_h\boldsymbol{\phi})+(P,\nabla\cdot(\boldsymbol{\phi}-I_h\boldsymbol{\phi}))\\
&+(\boldsymbol{F},\boldsymbol{\phi}-I_h\boldsymbol{\phi})+(\nabla\cdot\mathbf{U},z-\mathbb{P}_hz)
\end{aligned}$$

is the residual term.

6. Conclusions. We developed a preliminary *a posteriori* error analysis for the Lax-Friedrichs scheme applied to Burger's equation using the adjoint of the modified equation applied to the parabolic viscous Burgers equation, a scalar hydrodynamic model. We developed a preliminary analysis of the Lax-Friedrichs scheme for the hyperbolic inviscid Burgers equation and initiated an implementation for testing. We developed an *a posteriori* error estimate of the MAC scheme for the incompressible stationary Navier-Stokes hydrodynamic system in 2D and initiated an implementation of the adjoint solution for testing.

Through this project we have assessed that in the short term, it is not yet feasible to apply adjoint methods to hydrodynamic systems emitting discontinuities such as we have at LLNL. Further work is still required to mature tools such as modified equation analysis, variational forms, and viscous solutions for use within *a posteriori* error analysis for discretizations of hydrodynamic systems emitting discontinuities. We have established a collaboration between LLNL and Colorado State University and will continue adjoint method development for these systems through students and postdocs as well as through future proposals to LDRD and NSF.

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