



# Superconvergent functional output for time-dependent problems using finite differences on summation-by-parts form

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## ABSTRACT

Finite difference operators satisfying the summation-by-parts (SBP) rules can be used to obtain high order accurate, energy stable schemes for time-dependent partial differential equations, when the boundary conditions are imposed weakly by the simultaneous approximation term (SAT).

In general, an SBP-SAT discretization is accurate of order  $p + 1$  with an internal accuracy of  $2p$  and a boundary accuracy of  $p$ . Despite this, it is shown in this paper that any linear functional computed from the time-dependent solution, will be accurate of order  $2p$  when the boundary terms are imposed in a stable and dual consistent way.

The method does not involve the solution of the dual equations, and superconvergent functionals are obtained at no extra computational cost. Four representative model problems are analyzed in terms of convergence and errors, and it is shown in a systematic way how to derive schemes which gives superconvergent functional outputs.

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## 1. Introduction

When numerically computing solutions to equations in computational fluid dynamics (CFD), accurate solutions to the equations themselves might not be the primary target. Typically, functionals computed from the solution, such as the lift and drag coefficients, are of equal or even larger interest.

Already in the late 1990s, Giles et al. realized the importance of duality to enhance the computation of functionals in CFD applications [1–6]. Since then, duality and adjoint equations have been vastly studied in the context of finite element methods (FEM) [2] and more recently using discontinuous Galerkin (DG) methods [7–10], finite volume methods (FVM) [11] and spectral difference methods [12].

One can separate three distinct uses of the adjoint equations; adaptive mesh refinement [13], error analysis [14] and optimal design problems [15,16]. The success of duality based approaches to, in particular, adaptive mesh refinement and error estimation, has made the study of duality somewhat restricted to unstructured methods such as FEM, DG and FVM.

Recently, however, it was shown by Hicken and Zingg [17,18] that the adjoint equations can be used for finite difference (FD) methods to raise the order of accuracy of linear functionals computed from the FD solution. The technique was based on using FD operators on summation-by-parts (SBP) form [19,20] together with the simultaneous approximation term (SAT) for imposing boundary conditions weakly [21]. It was shown that when discretizing the equations in a dual consistent [9,17] way, the order of accuracy of the output functional was higher than the FD solution itself. This superconvergent behaviour

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was seen already in [3] for FEM and in [7] for DG, but it had not been previously proven for finite difference schemes. Some work on solution superconvergence for FD-based methods, using mimetic operators, can be seen in i.e. [22].

So far, most applications of the adjoint equations deal with steady-state problems, including the recent results presented in [17]. The reason is that the adjoint equation has limited use for realistic (non-linear) time-dependent problems since it runs backwards in time [23]. Hence to actually solve the adjoint time-dependent equation, the full time history of the primal equation has to be stored [24]. For large scale problems, this quickly becomes unfeasible [25,26]. Some work has been done in the time-dependent setting [25,23], in particular for adaptive error control [24,11,27] and optimization [26,12].

What is to be presented in this paper is the extension of [17] to unsteady problems for computing superconvergent time-dependent linear functionals. By superconvergence, we mean that the order of convergence of the output functional is higher than the design order of accuracy of the scheme. We will address two problems which usually occurs when attempting to use duality for time-dependent functional computations;

- The discrete adjoint equations does not approximate the continuous adjoint equations, i.e. the scheme is dual inconsistent
- If the scheme is dual consistent, it is unstable

The SBP discretization together with the SAT technique is highly suitable for addressing the above issues since the scheme allows for a multitude of parameters which can be chosen such that the scheme is both dual consistent and stable. These two features will result in a superconvergent time-dependent functional output.

## 2. SBP-SAT discretizations

Summation-by-parts finite difference operators were originally constructed by Kreiss and Scherer [28] in the 70's as a means for constructing energy stable [29] finite difference approximations. The operators are constructed such that they are automatically stable for linearly well-posed Cauchy problems. Together with the SAT procedure introduced by Carpenter et al. [21], the SBP-SAT technique provides a method of constructing energy stable and high order accurate finite difference schemes for any linearly well-posed initial-boundary value problem. Since then, the technique has been widely used and proven robust for a variety of problem. See for example [30–37] and references therein.

The SBP operators can be defined as follows.

**Definition 1.** A matrix  $D$  is called a first derivative SBP operator if  $D$  can be written as

$$D = P^{-1}Q, \quad (1)$$

where  $P$  defines a norm by  $\|u\|^2 = u^T P u$  and  $Q$  satisfies

$$Q + Q^T = \text{diag}[-1, 0, \dots, 0, 1]. \quad (2)$$

In this paper, only diagonal matrices  $P$  will be used. In that case,  $D$  consist of a  $2p$ -order accurate central difference approximation in the interior while at the boundaries, the accuracy reduces to a  $p$ -order one-sided difference. The global accuracy can then be shown to be  $p + 1$  [32].

By using non-diagonal matrices  $P$  as norms in the SBP definition, it is possible to raise both the boundary and global order of accuracy. For a block-diagonal  $P$ , the boundary stencil can be chosen to be  $2p - 1$  order accurate which increases the global accuracy to  $2p$  [19,32,38,39]. There are, however, drawbacks with a non-diagonal matrix  $P$ . In many cases, the equations are non-linear or have variable coefficients and energy stability can only be proven if  $P$  commutes with diagonal matrices. Unless  $P$  is carefully constructed to fit each problem under consideration, a diagonal  $P$  is the only alternative.

For many realistic problems, the boundary of the domain is non-smooth and the domain has to be split into blocks, where a curvilinear coordinate transformation is applied in each block. If the matrix  $P$  is not diagonal, energy stability cannot be shown in general since  $P$  is required to commute with the (diagonal) Jacobian matrix of the coordinate transformation [35,40–42].

When computing linear functionals, however, we can recover the loss compared to the accuracy from a non-diagonal  $P$ , while keeping the simplicity and flexibility of a diagonal  $P$ . It is hence always possible to prove energy stability, and keeping the full order of accuracy.

Currently there exist diagonal norm SBP operators for the first derivative accurate of order 2, 3, 4 and 5. The second derivative can be approximated using either the first derivative twice which results in a wide finite difference stencil, or a compact operator as described in [20,43]. In this paper, we will rewrite the equations in a form which does not require the application of a second derivative operator.

A first order hyperbolic PDE, for example the advection equation on  $0 \leq x \leq 1$ ,

$$\begin{aligned} u_t + au_x &= 0, \\ u(0, t) &= d_1(t), \\ u(x, 0) &= d_2(x), \end{aligned} \quad (3)$$

with  $a > 0$ , can be approximated on an equidistant grid with  $N + 1$  gridpoints as

$$\frac{d}{dt}u_h + aDu_h = 0, \quad (4)$$

where  $u_h$  is the discrete gridfunction approximating  $u$ . However, since the continuous PDE (3) needs to be supplied with a boundary condition at the inflow boundary, the scheme (4) has to be modified. The imposition of the boundary condition is done weakly using SAT as

$$\frac{d}{dt}u_h + aDu_h = \sigma P^{-1}(e_0^T u_h - d_1)e_0, \quad (5)$$

where  $e_0 = [1, 0, \dots, 0]$  and  $d_1 = d_1(t)$  is the time-dependent boundary data. The coefficient  $\sigma$  is a parameter which has to be determined such that the scheme is stable in the  $P$ -norm.

### 2.1. The energy method

To prove well-posedness of the continuous Eq. (3) and stability of the numerical scheme (5), the energy method in continuous and discrete form is used. We multiply (3) with  $u$  and integrate by parts over the spatial domain to obtain (when assuming  $d_1 = 0$ )

$$\|u\|_t^2 = -au^2(1, t). \quad (6)$$

It is clear that the growth rate of energy is bounded and hence we say that (3) is well-posed.<sup>1</sup>

In the discrete case we multiply (5) with  $u_h^T P$  and use the SBP properties of the operator to obtain

$$\|u_h\|_t^2 = (a + 2\sigma)u_h^2(x_0) - au_h^2(x_N). \quad (7)$$

It is clear that an energy estimate is obtained for

$$\sigma \leq -\frac{a}{2} \quad (8)$$

and for  $\sigma = -\frac{a}{2}$  we have exactly (6).

We can see that the parameter  $\sigma$  is allowed to vary in a semi-infinite range for which the scheme is stable. Any additional requirement we place on the scheme, for example dual consistency, has to be within a subset of values allowed by the energy estimate. This flexibility together with the ability to mimic integration by parts is what makes the SBP-SAT method suitable for treating adjoint problems.

**Remark 2.1.** Note that the assumption  $d_1 = 0$  merely simplifies the analysis. Boundary and initial data can be included, in which case the problem is called strongly well-posed. If the boundary and initial data is included in the discrete case, and an energy estimate is obtained, the problem is called strongly stable [45].

## 3. Adjoint problems and dual consistency

There are various ways of obtaining the adjoint equations. Most common is to consider a PDE subject to a set of control parameters and a functional output of interest, and in various ways taking derivatives of the functional with respect to the control parameters [1,27]. The adjoint equation can then be seen as a sensitivity equation for the primal PDE, and is sometimes referred to as the sensitivity equation. In this work we will adopt the notation in [17] and derive the adjoint equation by posing the SBP-SAT method in a variational framework similar to the one used in FEM.

The order of convergence is measured in space, not in time. To obtain a superconvergent time-dependent linear functional output, it is sufficient to consider the steady equations and discretize them in a dual consistent way which does not violate any stability conditions for the unsteady equations.

We shall use the following notations regarding the inner products. The continuous inner product is defined as

$$(f, g) = \int_{\Omega} fgd\Omega \quad (9)$$

and the corresponding discrete inner product is defined as

$$(f_h, g_h)_h = f_h^T P g_h, \quad (10)$$

where  $f_h, g_h$  are projections of  $f, g$  onto a grid, and  $P$  is the matrix (and integration operator) used to define a norm in the definition of the SBP operator. The subscript  $h$  will be omitted for known functions if the meaning is clear from the context.

Before we begin, we need to define what is meant by the continuous dual problem, discrete dual problem and dual consistency. Let  $L$  be a linear differential operator and consider the (steady) equation

<sup>1</sup> Existence of solutions is not formally considered in this context. Existence is motivated by the fact that a minimal number of boundary conditions is used to obtain an energy estimate [44].

$$Lu - f = 0, \quad \forall x \in \Omega, \quad (11)$$

subject to homogeneous boundary conditions. Let

$$J(u) = (g, u) \quad (12)$$

be a linear functional output of interest. We obtain the adjoint equation by seeking  $\phi$  in some appropriate function space, such that

$$J(u) = (\phi, f). \quad (13)$$

A formal computation gives

$$J(u) = (g, u) - (\phi, Lu - f) = (\phi, f) - (L^* \phi - g, u) \quad (14)$$

and hence the adjoint equation is given by

$$L^* \phi - g = 0, \quad (15)$$

where  $L^*$  is the formal adjoint of  $L$ . Note that  $L^*$  is abstractly defined, and finding an exact expression for the dual operator is in general a non-trivial task. In the case of linear differential operators, the adjoint operator is obtained by integration by parts.

**Remark 3.1.** In this paper, we consider homogeneous boundary and initial conditions. This is only for the purpose of analysis. The dual problem depends only on the form of the boundary conditions, but not on the particular boundary or initial data. In computations, the boundary and initial data can be non-zero.

The boundary conditions for the adjoint equation are obtained by considering the boundary terms resulting from the integration by parts procedure. After applying the homogeneous boundary conditions for the primal PDE, the dual boundary conditions are defined as the minimal set of homogeneous conditions such that all boundary terms vanish.

**Definition 2.** The *continuous dual problem* is given by

$$L^* \phi = g \quad (16)$$

subject to the dual boundary conditions.

The same reasoning can be applied in the discrete setting. Let

$$L_h u_h - f = 0 \quad (17)$$

be a discretization of (11), including the homogeneous boundary conditions. Then

$$J_h(u_h) = (g, u_h)_h \quad (18)$$

is an approximation of (12). We obtain the discrete dual problem by seeking  $\phi_h$  such that

$$J_h(u_h) = (\phi_h, f)_h. \quad (19)$$

The same formal computation as before gives

$$J_h(u_h) = (g, u_h)_h - (\phi_h, L_h u_h - f)_h = (\phi_h, f)_h - (P^{-1} L_h^T P \phi_h - g, u_h)_h \quad (20)$$

and we have

**Definition 3.** The *discrete dual problem* is given by

$$P^{-1} L_h^T P \phi_h - g = 0. \quad (21)$$

**Remark 3.2.** In an SBP-SAT setting, the difference operator  $L_h$  can be written as

$$L_h = P^{-1} \tilde{L}_h \quad (22)$$

and the discrete dual problem reduces to

$$P^{-1} \tilde{L}_h^T \phi_h = g. \quad (23)$$

Finally, by using (16) and (21) we make the definition of dual consistency.

**Definition 4.** A discretization is called *dual consistent* if (21) is a consistent approximation of (16).

So far, we have been concerned with steady problems only. Since we are interested in unsteady problems, we need to define what is meant by dual consistency in this context. Consider an unsteady problem

$$u_t + Lu - f = 0, \quad t > 0, \quad \forall x \in \Omega, \quad (24)$$

subject to homogeneous boundary and initial conditions. By seeking  $\phi$  such that

$$\int_0^T J(u) dt = \int_0^T (\phi, f) dt \quad (25)$$

we obtain

$$\begin{aligned} \int_0^T J(u) dt &= \int_0^T J(u) dt - \int_0^T (\phi, u_t + Lu - f) dt \\ &= \int_0^T (\phi_t - L^* \phi + g, u) dt + \int_0^T (\phi, f) dt. \end{aligned} \quad (26)$$

The time-dependent dual problem thus becomes

$$-\phi_t + L^* \phi = g \quad (27)$$

subject to the dual boundary conditions. A homogeneous initial condition for the dual problem is placed at time  $t = T$  which removes the boundary term from the partial time integration.

The discrete procedure can be formulated analogously. Let

$$\frac{d}{dt} u_h + L_h u_h - f = 0 \quad (28)$$

be a semi-discretization of (24), including the boundary conditions. We then have the following definition regarding dual consistency of time-dependent problems,

**Definition 5.** The semi-discretization (28) is called *spatially dual consistent* if the corresponding steady problem is dual consistent.

Note that a stable and consistent discretization of the primal PDE does not imply spatial dual consistency.

To prove the main result of this paper, we need Corollary 1 from [46], which states that  $P$  is a  $2p$ -order accurate quadrature. For our purpose, we can restate the result as.

**Lemma 3.1.** Let  $P$  be the norm-matrix of an SBP discretization with  $2p$ -order internal accuracy. Then for  $u \in C^{2p}$  we have

$$J_h(u) = J(u) + O(h^{2p}). \quad (29)$$

Using Lemma 3.1 we can prove the main result of this paper which is.

**Theorem 3.2.** Let

$$\frac{d}{dt} u_h + L_h u_h = f \quad (30)$$

be a stable and spatial dual consistent SBP-SAT discretization of the continuous problem

$$u_t + Lu = f. \quad (31)$$

Then the linear functional

$$J_h(u_h) = g^T P u_h \quad (32)$$

is a  $2p$ -order accurate approximation of

$$J(u) = \int_{\Omega} g^T u d\Omega. \quad (33)$$

**Proof.** By using the results in [46] together with the definition of the discrete dual problem, we can add and subtract terms to relate the the continuous functional to the discrete as

$$\begin{aligned} J(u) &= J_h(u) + O(h^{2p}) = g^T P u_h + g^T P(u - u_h) + O(h^{2p}) = g^T P u_h + g^T P(u - u_h) - \phi_h^T P(L_h u_h - f) + O(h^{2p}) \\ &= J_h(u_h) + g^T P(u - u_h) - \phi_h^T P L_h(u - u_h) - \phi_h^T P f + \phi_h^T P L_h u + O(h^{2p}) \\ &= J_h(u_h) - (u - u_h)^T P(P^{-1} L_h^T P \phi_h - g) + \phi_h^T P(L_h u - f) + O(h^{2p}) = J_h(u_h) + \phi_h^T P(L_h u - f) + O(h^{2p}), \end{aligned} \quad (34)$$

where the last error term is of order  $h^{2p}$  [46]. We can hence conclude that

$$J(u) = J_h(u_h) + O(h^{2p}). \quad \square \quad (35)$$

#### 4. Derivation of stable and spatially dual consistent schemes

Based on Theorem 3.2, we will derive stable and spatially dual consistent schemes for four time-dependent model problems in a systematic way. The equations we consider are the advection equation, the heat equation, the viscous Burgers' equation and an incompletely parabolic system of equations. We will see that a stable and spatial dual consistent discretization produces superconvergent time-dependent linear functionals.

##### 4.1. The advection equation

Consider (3) again together with a linear functional output of interest. We let the boundary condition be homogeneous, add a forcing function and ignore the initial condition,

$$\begin{aligned} u_t + au_x &= f, \\ u(0, t) &= 0, \\ J(u) &= (g, u). \end{aligned} \quad (36)$$

Note that  $J(u)$  is a time-dependent functional. The adjoint equation is obtained by letting  $u_t = 0$  and finding  $\phi$  such that  $J(u) = (\phi, f)$ . We get

$$J(u) = J(u) - \int_0^1 \phi(au_x - f)dx = -a\phi(1, t)u(1, t) - \int_0^1 (g + a\phi_x)u dx + (v, f) \quad (37)$$

and hence the steady adjoint problem is given by

$$\begin{aligned} -a\phi_x &= g, \\ \phi(1, t) &= 0. \end{aligned} \quad (38)$$

Note that the sign has changed and the adjoint boundary condition is located at the opposite boundary compared to the primal problem.

Eq. (36) is discretized as before,

$$\frac{d}{dt}u_h + aP^{-1}Qu_h = f + \sigma P^{-1}(e_0^T u_h - \mathbf{0})e_0, \quad (39)$$

where  $\mathbf{0}$  is the boundary data. We know from the preceding energy estimate (7) that the scheme is stable if  $\sigma \leq -\frac{a}{2}$ . The addition of the forcing function does not change the number or form of the boundary conditions and can be assumed to be zero in an energy estimate according to the principle of Duhamel [45]. To determine spatial dual consistency, we let  $\frac{d}{dt}u_h = 0$  and rewrite (39) as

$$L_h u_h = Pf, \quad (40)$$

where

$$L_h = aQ - \sigma E_0 \quad (41)$$

and  $E_0 = e_0^T e_0 = \text{diag}[1, 0, \dots, 0]$ . According to the definition of dual consistency,

$$L_h^T \phi_h = Pg \quad (42)$$

has to be a consistent approximation of the adjoint Eq. (38). By using the SBP property of  $Q$ , we expand (42) as

$$-aP^{-1}Q\phi_h = g - aP^{-1}E_N\phi_h + (\sigma + a)P^{-1}E_0\phi_h \quad (43)$$

which is a consistent approximation of (38) only if

$$\sigma = -a. \quad (44)$$

For any other value of  $\sigma$ , the numerical scheme would impose a boundary condition at  $x = 0$  which does not exist in the adjoint equation. We can also see that  $\sigma = -a$  does not violate the stability condition given by the energy estimate. Thus the scheme is both stable and spatially dual consistent.

**Remark 4.1.** Note that the parameter  $\sigma$  is allowed to vary in a semi-infinite range from the stability requirements, while spatial dual consistency requires a unique value.

##### 4.2. The heat equation

The heat equation on  $0 \leq x \leq 1$  with homogeneous Dirichlet boundary conditions is given by

$$\begin{aligned}
u_t &= \alpha u_{xx} + f, \\
u(0, t) &= 0, \\
u(1, t) &= 0, \\
J(u) &= (g, u).
\end{aligned} \tag{45}$$

The initial condition is omitted since the derivation of the dual problem depends only on the equation and the form of the boundary conditions. In the computations, however, an initial condition has to be supplied. In order to derive a stable and spatially dual consistent scheme, (45) has to be rewritten as a first order system in the same way as in the local discontinuous Galerkin (LDG) method [47]. It has been shown that the LDG method has interesting superconvergent features not only for functionals, but also for the solution itself [7,30,48]. We hence adapt the LDG formulation and rewrite (45) as

$$\begin{aligned}
u_t &= \sqrt{\alpha} v_x + f, \\
v &= \sqrt{\alpha} u_x, \\
u(0, t) &= 0, \\
u(1, t) &= 0, \\
J(u) &= (g, u).
\end{aligned} \tag{46}$$

To obtain the dual problem, we let  $u_t = 0$  and write (46) as

$$Aw + Bw_x = F, \tag{47}$$

where  $w = [u, v]^T$ ,  $F = [f, 0]^T$  and

$$A = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & -\sqrt{\alpha} \\ -\sqrt{\alpha} & 0 \end{bmatrix}. \tag{48}$$

Let now  $G = [g, 0]^T$ ,  $\theta = [\phi, \psi]^T$  and find  $\theta$  such that

$$J(w) = (\theta, F). \tag{49}$$

Note that

$$J(w) = (G, w) = (g, u) \tag{50}$$

and we are still computing the functional of interest from the primal problem. This gives us the adjoint problem by computing

$$J(w) = J(w) - \int_0^1 \theta^T (Aw + Bw_x - F) dx = \int_0^1 w^T (G - A\theta + B\theta_x) dx - [\theta^T Bw]_0^1 + (\theta, F). \tag{51}$$

The adjoint equation is thus given by

$$A\theta - B\theta_x = G \tag{52}$$

and the adjoint boundary conditions are the minimal number of conditions such that  $[\theta^T Bw]_0^1 = 0$ . After applying the homogeneous boundary conditions for the primal problem, we get the adjoint problem on component form

$$\begin{aligned}
\sqrt{\alpha} \psi_x &= g, \\
\psi + \sqrt{\alpha} \phi_x &= 0, \\
\phi(0, t) &= 0, \\
\phi(1, t) &= 0.
\end{aligned} \tag{53}$$

The primal PDE on LDG form (46) is discretized as

$$\begin{aligned}
\frac{d}{dt} u_h &= \sqrt{\alpha} P^{-1} Q v_h + f + \sigma_L P^{-1} (e_0^T u_h - \mathbf{0}) e_0 + \sigma_R P^{-1} (e_N^T u_h - \mathbf{0}) e_N, \\
v_h &= \sqrt{\alpha} P^{-1} Q u_h + \tau_L P^{-1} (e_0^T u_h - \mathbf{0}) e_0 + \tau_R P^{-1} (e_N^T u_h - \mathbf{0}) e_N.
\end{aligned} \tag{54}$$

By multiplying the first equation by  $u_h^T P$ , the second by  $v_h^T P$  and adding the results we get

$$\frac{1}{2} \frac{d}{dt} \|u_h\|^2 + \|v_h\|^2 = (\tau_L - \sqrt{\alpha}) u_h^T E_0 v_h + (\tau_R + \sqrt{\alpha}) u_h^T E_N v_h + \sigma_L u_h^T E_0 u_h + \sigma_R u_h^T E_N u_h \tag{55}$$

and the scheme is clearly stable if

$$\tau_L = \sqrt{\alpha}, \quad \tau_R = -\sqrt{\alpha}, \quad \sigma_L \leq 0, \quad \sigma_R \leq 0. \tag{56}$$

To determine spatial dual consistency we again let  $u_t = 0$  and rewrite (54), using (56), as

$$L_h w_h = \tilde{F}, \quad (57)$$

where  $w_h = [u_h, v_h]^T$ ,  $\tilde{F} = [Pf, 0]^T$  and

$$L_h = \begin{bmatrix} -\sigma_L E_0 - \sigma_R E_N & -\sqrt{\alpha} Q \\ -\sqrt{\alpha} Q - \sqrt{\alpha} E_0 + \sqrt{\alpha} E_N & P \end{bmatrix}. \quad (58)$$

The discrete dual problem is given by

$$L_h^T \theta_h = \tilde{G}, \quad (59)$$

where  $\theta_h = [\phi_h, \psi_h]^T$ ,  $\tilde{G} = [Pg, 0]^T$ , and it has to be a consistent approximation of (53) without violating the stability conditions (56). By using the SBP properties of the operators we expand (59) and write it in component form as

$$\begin{aligned} \sqrt{\alpha} P^{-1} Q \psi_h &= g + \sigma_L P^{-1} E_0 \phi_h + \sigma_R P^{-1} E_N \phi_h \\ \psi_h + \sqrt{\alpha} P^{-1} Q \phi_h &= -\sqrt{\alpha} P^{-1} E_0 \phi_h + \sqrt{\alpha} P^{-1} E_N \phi_h \end{aligned} \quad (60)$$

which exactly approximates (53), including the dual boundary conditions. Note that there are no restrictions on  $\sigma_{L,R}$  for dual consistency.

**Remark 4.2.** Note that the stability requirements are sufficient for spatial dual consistency, in contrast to the pure advection case.

**Remark 4.3.** The LDG form can be transformed back to second order form, see also [30], in which case the scheme becomes

$$\frac{d}{dt} u_h = \alpha (P^{-1} Q)^2 u_h + f + (\sigma_L I + \alpha P^{-1} Q) P^{-1} (e_0^T u_h - \mathbf{0}) e_0 + (\sigma_R I - \alpha P^{-1} Q) P^{-1} (e_N^T u_h - \mathbf{0}) e_N, \quad (61)$$

where  $I$  is the identity matrix of size  $N + 1$ . Note that we get back the wide second derivative operator, possibly suggesting that dual consistency requires a second derivative operator which can be factorized into the product of two first derivative operators.

#### 4.3. The viscous Burgers' equation

The viscous Burgers' equation, together with a linear functional of interest, with homogeneous Dirichlet boundary conditions on  $0 \leq x \leq 1$  is given on conservative form by

$$\begin{aligned} u_t + \left( \frac{u^2}{2} \right)_x &= \varepsilon u_{xx} + f, \\ u(0, t) &= 0, \\ u(1, t) &= 0, \\ J(u) &= (g, u). \end{aligned} \quad (62)$$

Since (62) is a non-linear equation, the present theory cannot directly be applied. The viscous Burger's equation have regular solutions due to the viscosity term, and the behavior of the solution is not far from that of a linear problem. In the absence of a general method for non-linear analysis, a linear analysis is used. In the presence of shocks, for more complicated equations, it is not clear what meaning a linear analysis have.

We linearize (62) around a constant state  $u = a$  to obtain the linear equation,

$$\begin{aligned} u_t + a u_x &= \varepsilon u_{xx} + f, \\ u(0, t) &= 0, \\ u(1, t) &= 0, \\ J(u) &= (g, u), \end{aligned} \quad (63)$$

which is usually referred to as the advection–diffusion equation.

Since (62) contains second derivatives, we introduce the auxiliary variable  $v = \sqrt{\varepsilon} u_x$  and rewrite the steady (linear) problem as

$$Aw + Bw_x = F, \quad (64)$$

where  $w = [u, v]^T$ ,  $F = [f, 0]^T$  and

$$A = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} a & -\sqrt{\varepsilon} \\ -\sqrt{\varepsilon} & 0 \end{bmatrix}. \quad (65)$$



To find the adjoint equation, we define  $G = [g, 0]^T$  and seek  $\theta = [\phi, \psi]^T$  such that

$$J(w) = (\theta, F) \quad (66)$$

as before. Integration by parts leads to

$$J(w) = J(w) - \int_0^1 \theta^T (Aw + Bw_x - F) dx = \int_0^1 w^T (G - A\theta + B\theta_x) dx - [\theta^T Bw]_0^1 + (\theta, F) \quad (67)$$

and hence the adjoint equation is given on component form as

$$\begin{aligned} -a\phi_x + \sqrt{\varepsilon}\psi_x &= g, \\ \phi + \sqrt{\varepsilon}\phi_x &= 0, \\ \phi(0, t) &= 0, \\ \phi(1, t) &= 0. \end{aligned} \quad (68)$$

The stability analysis will also be performed on the linearized equations. The time-dependent equation on LDG form is discretized as

$$\begin{aligned} \frac{d}{dt} u_h + aP^{-1}Qu_h &= \sqrt{\varepsilon}P^{-1}Qv_h + \sigma_L P^{-1}(e_0^T u_h - \mathbf{0})e_0 + \sigma_R P^{-1}(e_N^T u_h - \mathbf{0})e_N + f, \\ v_h &= \sqrt{\varepsilon}P^{-1}Qu_h + \tau_L P^{-1}(e_0^T u_h - \mathbf{0})e_0 + \tau_R P^{-1}(e_N^T u_h - \mathbf{0})e_N \end{aligned} \quad (69)$$

and the coefficients  $\sigma_{L,R}$  and  $\tau_{L,R}$  has to be determined such that the scheme is stable. By multiplying the first equation in (69) by  $u_h^T P$  and the second by  $v_h^T P$ , we obtain by adding the results

$$\frac{d}{dt} \|u_h\|^2 + 2\|v_h\|^2 = (2\sigma_L + a)u_h^T E_0 u_h + (2\sigma_R - a)u_h^T E_N u_h + 2(\tau_L - \sqrt{\varepsilon})v_h^T E_0 u_h + 2(\tau_R + \sqrt{\varepsilon})v_h^T E_N u_h. \quad (70)$$

We can see that (70) is stable if we chose

$$\sigma_L \leq -\frac{a}{2}, \quad \sigma_R \leq \frac{a}{2}, \quad \tau_L = \sqrt{\varepsilon}, \quad \tau_R = -\sqrt{\varepsilon}. \quad (71)$$

To determine if the scheme is spatially dual consistent, we let  $u_t = 0$  and rewrite (69), using (71), as

$$L_h w_h = \tilde{F}, \quad (72)$$

where  $w_h = [u_h, v_h]^T$ ,  $\tilde{F} = [Pf, 0]^T$  and

$$L_h = \begin{bmatrix} aQ + \sigma_L E_0 + \sigma_R E_N & -\sqrt{\varepsilon} \\ -\sqrt{\varepsilon}Q - \sqrt{\varepsilon}E_0 + \sqrt{\varepsilon}E_N & P \end{bmatrix}. \quad (73)$$

The discrete dual problem is then given by

$$L_h^T \theta_h = \tilde{G}, \quad (74)$$

where  $\theta_h = [\phi_h, \psi_h]^T$  and  $\tilde{G} = [Pg, 0]^T$ , which has to be a consistent approximation of (68) without violating the stability conditions (71). By expanding (74), we can write it in component form as

$$\begin{aligned} -aP^{-1}Q\phi_h + \sqrt{\varepsilon}P^{-1}Q\psi_h &= -(\sigma_L - a)P^{-1}E_0\phi_h - (\sigma_R + a)P^{-1}E_N\phi_h + g \\ \psi_h + \sqrt{\varepsilon}P^{-1}Q\phi_h &= -\sqrt{\varepsilon}P^{-1}E_0\phi_h + \sqrt{\varepsilon}P^{-1}E_N\phi_h \end{aligned} \quad (75)$$

which can be seen to be a consistent approximation of (74) without violating any of the stability conditions in (71). Hence the scheme (69) is both a stable and spatially dual consistent approximation of the linearized equation.

When performing the computations, however, we use the nonlinear LDG formulation

$$\begin{aligned} \frac{d}{dt} u_h + P^{-1}Q\left(\frac{u_h^2}{2}\right) &= \sqrt{\varepsilon}P^{-1}Qv_h + \sigma_L P^{-1}(e_0^T u_h - \mathbf{0})e_0 + \sigma_R P^{-1}(e_N^T u_h - \mathbf{0})e_N + f, \\ v_h &= \sqrt{\varepsilon}P^{-1}Qu_h + \tau_L P^{-1}(e_0^T u_h - \mathbf{0})e_0 + \tau_R P^{-1}(e_N^T u_h - \mathbf{0})e_N, \end{aligned} \quad (76)$$

where every occurrence of the mean flow coefficient,  $a$ , in the SAT is replaced by  $u$  to obtain a nonlinear SAT. This procedure is motivated by the linearization and localization principle, see [49] for details.

**Remark 4.4.** Note again that stability is sufficient for spatial dual consistency and no extra conditions have to be placed on the SAT coefficients. The coefficients  $\sigma_{L,R}$  are still allowed to vary in a semi-infinite range.

#### 4.4. An incompletely parabolic system

In this section we consider the incompletely parabolic system

$$\begin{aligned} U_t + AU_x &= BU_{xx} + F, \\ J(U) &= (G, U), \end{aligned} \quad (77)$$

where  $U = [p, u]^T$ ,  $F = [f_1, f_2]^T$ ,  $G = [g_1, g_2]^T$  and

$$A = \begin{bmatrix} \bar{u} & \bar{c} \\ \bar{c} & \bar{u} \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 \\ 0 & \varepsilon \end{bmatrix}. \quad (78)$$

Eq. (77) can be thought of as the symmetrized [50] Navier–Stokes equations linearized around the mean velocity  $\bar{u} > 0$  and speed of sound  $\bar{c}$ . We shall assume a linearization around a subsonic flow field, that is  $\bar{u} < \bar{c}$ . In this case, (77) requires two boundary conditions at the inflow boundary and one at the outflow. For the purpose of analysis, we will use the homogeneous Dirichlet conditions

$$u(0, t) = 0, \quad p(0, t) = 0, \quad u(1, t) = 0. \quad (79)$$

To obtain the adjoint equations, we let  $u_t = p_t = 0$  and rewrite (77) in LDG form as

$$\bar{A}w + \bar{B}w_x = \bar{F}, \quad (80)$$

where  $w = [p, u, v]^T$ ,  $\bar{F} = [f_1, f_2, 0]^T$ ,  $v = \sqrt{\varepsilon}u_x$  and

$$\bar{A} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \bar{B} = \begin{bmatrix} \bar{u} & \bar{c} & 0 \\ \bar{c} & \bar{u} & -\sqrt{\varepsilon} \\ 0 & -\sqrt{\varepsilon} & 0 \end{bmatrix}. \quad (81)$$

The adjoint equations are now found by seeking  $\theta = [\phi, \psi, v]^T$  such that

$$J(w) = (\theta, \bar{F}). \quad (82)$$

Integration by parts gives

$$J(w) = J(w) - \int_0^1 \theta^T (\bar{A}w + \bar{B}w_x - \bar{F}) dx = \int_0^1 w^T (\bar{G} - \bar{A}\theta + \bar{B}\theta_x) dx - [\theta^T \bar{B}w]_0^1 + (\theta, \bar{F}), \quad (83)$$

where  $\bar{G} = [g_1, g_2, 0]^T$ . The adjoint problem is hence given on component form as

$$\begin{aligned} -\bar{u}\phi_x - \bar{c}\psi_x &= g_1, \\ -\bar{c}\phi_x - \bar{u}\psi_x + \sqrt{\varepsilon}v_x &= g_2, \\ v + \sqrt{\varepsilon}\psi_x &= 0, \\ \psi(0, t) &= 0, \\ \phi(1, t) &= 0, \\ \psi(1, t) &= 0. \end{aligned} \quad (84)$$

Note that the dual problem has one boundary condition at  $x = 0$  and two at  $x = 1$ , in contrast to the primal problem for which the situation is reversed.

The time-dependent problem (80) is discretized as

$$\begin{aligned} \frac{d}{dt} p_h + \bar{u}P^{-1}Qp_h + \bar{c}P^{-1}Qu_h &= \sigma_1 P^{-1}(e_0^T p_h - \mathbf{0})e_0 + \sigma_2 P^{-1}(e_0^T u_h - \mathbf{0})e_0 + \sigma_3 P^{-1}(e_N^T u_h - \mathbf{0})e_N, \\ \frac{d}{dt} u_h + \bar{c}P^{-1}Qp_h + \bar{u}P^{-1}Qu_h - \sqrt{\varepsilon}P^{-1}Qv_h &= \tau_1 P^{-1}(e_0^T p_h - \mathbf{0})e_0 + \tau_2 P^{-1}(e_0^T u_h - \mathbf{0})e_0 + \tau_3 P^{-1}(e_N^T u_h - \mathbf{0})e_N, \\ v_h - \sqrt{\varepsilon}P^{-1}Qu_h &= \gamma_1 P^{-1}(e_0^T p_h - \mathbf{0})e_0 + \gamma_2 P^{-1}(e_0^T u_h - \mathbf{0})e_0 + \gamma_3 P^{-1}(e_N^T u_h - \mathbf{0})e_N \end{aligned} \quad (85)$$

and the coefficients  $\sigma_{1,2,3}$ ,  $\tau_{1,2,3}$  and  $\gamma_{1,2,3}$  has to be determined such that the scheme is stable. By applying the energy method to each of the equations and adding them, we can write the result as

$$\frac{d}{dt} \|p_h\|^2 + \frac{d}{dt} \|u_h\|^2 + 2\|v_h\|^2 = w_h^T M_0 w + w_h^T M_N w, \quad (86)$$

where  $w_h = [p_h, u_h, v_h]$  and

$$M_0 = \begin{bmatrix} (\bar{u} + 2\sigma_1)E_0 & (\bar{c} + \sigma_2 + \tau_1)E_0 & \gamma_1 E_0 \\ (\bar{c} + \sigma_2 + \tau_1)E_0 & (\bar{u} + 2\tau_2)E_0 & (\gamma_2 - \sqrt{\varepsilon})E_0 \\ \gamma_1 E_0 & (\gamma_2 - \sqrt{\varepsilon})E_0 & 0 \end{bmatrix}, \quad (87)$$

$$M_N = \begin{bmatrix} -\bar{u}E_N & (-\bar{c} + \sigma_3)E_N & 0 \\ (-\bar{c} + \sigma_3)E_N & (-\bar{u} + 2\tau_3)E_N & (\gamma_3 + \sqrt{\varepsilon})E_N \\ 0 & (\gamma_3 + \sqrt{\varepsilon})E_N & 0 \end{bmatrix}.$$

To simplify (86), we introduce the Kronecker product, which is defined for arbitrary matrices  $X$  and  $Y$  by

$$X \otimes Y = \begin{bmatrix} x_{11}Y & x_{12}Y & \dots & x_{1n}Y \\ x_{21}Y & x_{22}Y & \dots & x_{2n}Y \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1}Y & x_{m2}Y & \dots & x_{mn}Y \end{bmatrix}. \quad (88)$$

The Kronecker product is bilinear, associative and satisfies the mixed product property

$$(X_1 \otimes Y_1)(X_2 \otimes Y_2) = (X_1 X_2 \otimes Y_1 Y_2) \quad (89)$$

if the usual matrix products are defined. For inversion and transposing we have

$$(X \otimes Y)^{-1,T} = (X^{-1,T} \otimes Y^{-1,T}) \quad (90)$$

if the usual matrix inverses are defined.

Using the Kronecker product, we can factorize (86) as

$$\frac{d}{dt} \|p_h\|^2 + \frac{d}{dt} \|u_h\|^2 + 2\|v_h\|^2 = w_h^T (m_0 \otimes E_0) w_h + w_h^T (m_N \otimes E_N) w_h, \quad (91)$$

where  $m_{0,N}$  are the smaller submatrices

$$m_0 = \begin{bmatrix} \bar{u} + 2\sigma_1 & \bar{c} + \sigma_2 + \tau_1 & \gamma_1 \\ \bar{c} + \sigma_2 + \tau_1 & \bar{u} + 2\tau_2 & \gamma_2 - \sqrt{\varepsilon} \\ \gamma_1 & \gamma_2 - \sqrt{\varepsilon} & 0 \end{bmatrix}, \quad (92)$$

$$m_N = \begin{bmatrix} -\bar{u} & -\bar{c} + \sigma_3 & 0 \\ -\bar{c} + \sigma_3 & -\bar{u} + 2\tau_3 & \gamma_3 + \sqrt{\varepsilon} \\ 0 & \gamma_3 + \sqrt{\varepsilon} & 0 \end{bmatrix}. \quad (93)$$

Since  $E_0, E_N \geq 0$ , we obtain a stable scheme if the coefficients are chosen such that  $m_0, m_N \leq 0$ . The coefficients are given in

**Proposition 4.1.** *The scheme (85) is stable using*

$$\sigma_1 \leq -\frac{\bar{u}}{2}, \quad \bar{c} + \sigma_2 + \tau_1 = 0, \quad \tau_2 \leq -\frac{\bar{u}}{2}, \quad \gamma_1 = 0, \quad \gamma_2 = \sqrt{\varepsilon} \quad (94)$$

for the coefficients in (92) and

$$\sigma_3 = \bar{c}, \quad \gamma_3 = -\sqrt{\varepsilon}, \quad \tau_3 \leq \frac{\bar{u}}{2} \quad (95)$$

for the coefficients in (93).

**Proof.** By inserting the coefficients (94) and (95) into the scheme (85), the energy estimate (91) reduces to

$$\frac{d}{dt} \|p_h\|^2 + \frac{d}{dt} \|u_h\|^2 + 2\|v_h\|^2 \leq 0. \quad \square \quad (96)$$

To determine the spatial dual consistency of (85), we let  $p_t = u_t = 0$  and rewrite as

$$L_h w_h = \tilde{F}, \quad (97)$$

where  $\tilde{F} = [Pf_1, Pf_2, 0]^T$  and

$$L_h = \begin{bmatrix} \bar{u}Q - \sigma_1 E_0 & \bar{c}Q - \sigma_2 E_0 - \bar{c}E_N & 0 \\ \bar{c}Q - \tau_1 E_0 & \bar{u}Q - \tau_2 E_0 - \tau_3 E_N & -\sqrt{\varepsilon}Q \\ 0 & -\sqrt{\varepsilon}Q - \sqrt{\varepsilon}E_0 + \sqrt{\varepsilon}E_N & P \end{bmatrix}. \quad (98)$$

The discrete dual problem is then given by

$$L_h^T \theta_h = \tilde{G}, \quad (99)$$

where  $\theta_h = [\phi_h, \psi_h, v_h]^T$ ,  $\tilde{G} = [Pg_1, Pg_2, 0]^T$ , and it has to be a consistent approximation of (84) without violating the stability conditions. By expanding (99), using (94) and (95), we get

$$\begin{aligned} -\bar{u}P^{-1}Q\phi_h - \bar{c}P^{-1}Q\psi_h &= (\sigma_1 + \bar{u})P^{-1}E_0\phi_h + (\tau_1 + \bar{c})P^{-1}E_0\psi_h - \bar{u}P^{-1}E_N\phi_h - \bar{c}P^{-1}E_N\psi_h + g_1, \\ -\bar{c}P^{-1}Q\phi_h - \bar{u}P^{-1}Q\psi_h + \sqrt{\varepsilon}P^{-1}Qv_h &= (\sigma_2 + \bar{c})P^{-1}E_0\phi_h + (\tau_2 + \bar{u})P^{-1}E_0\psi_h + (\tau_3 - \bar{u})P^{-1}E_N\psi_h + g_2, \\ \sqrt{\varepsilon}P^{-1}Q\psi_h + v &= -\sqrt{\varepsilon}P^{-1}E_0\psi_h + \sqrt{\varepsilon}P^{-1}E_N\psi_h. \end{aligned} \quad (100)$$

Remember that the boundary conditions in the dual Eq. (84) are different from those of the primal equation. This puts restrictions on the coefficients in order to obtain a consistent approximation of the dual problem. The coefficients are given in

**Proposition 4.2.** *The scheme (85) is stable and spatially dual consistent with (94), (95) and the choices*

$$\sigma_1 = -\bar{u}, \quad \sigma_2 = -\bar{c}. \quad (101)$$

**Proof.** The choice (101) cancels the terms in (100) for which additional erroneous boundary conditions would be imposed for the dual problem. Note that  $\sigma_2 = -\bar{c}$  implies

$$\tau_1 = 0. \quad (102)$$

The choice of coefficients given in (101) and (102) does not violate the stability conditions given in (94) and (95).  $\square$

**Remark 4.5.** Note that only the coefficients at the inflow boundary are uniquely determined by the spatial dual consistency requirements. For the outflow boundary, the conditions for stability are sufficient.

**Remark 4.6.** The requirements for spatial dual consistency has always constituted a subset of the stability requirements. We have hence been able to construct schemes which are both energy stable and spatially dual consistent. The energy analysis for stability typically renders some coefficients in the SAT to be semi-bounded, while the additional requirement of spatial dual consistency fixes some coefficients to unique values in the semi-bounded region.

## 5. Numerical results

A forcing function have been chosen in all cases such that an analytical solution is known, and the rate of convergence and errors are computed with respect to the analytical solution. The analytical solution is smooth for all times, even for the viscous Burger's equation. This is known as the method of manufactured solutions [51]. Note that the boundary and initial data are constructed from the analytical solution and are hence the conditions are no longer homogeneous.

The time integration is performed until time  $t = 10$  using the classical 4th-order Runge–Kutta method with timestep  $\Delta t = 2 \times 10^{-6}$ , to ensure that the time integration errors are negligible. In each time step we perform a mesh refinement from 32 to 160 gridpoints, in steps of 16, and compute the rate of convergence for both the solution and the functional. In this way, the rate of convergence can be computed as a function of time.

We compare the new schemes with standard SBP–SAT schemes which impose the Dirichlet boundary conditions traditionally without respect to the dual problem. The solutions to all problems were verified to converge with the design order of accuracy. In Tables 1 and 2 we summarize the time-average rates of functional convergence for the dual consistent and dual inconsistent cases, respectively.

The advection equation, heat equation, viscous Burger's equation and the incompletely parabolic system of equations are representatives for the hyperbolic, parabolic, nonlinear and mixed type of partial differential equations. Despite them being different in nature, the results regarding the functional convergence are consistent. A spatially dual consistent SBP–SAT discretization gives rise to time-dependent superconvergent linear functional output.

**Table 1**

Time-average rates of the functional convergence for the dual consistent discretization.

Accuracy	Advection	Heat	Burger's	System $(J(p), J(u))$
3rd	4.14808	4.0073	4.19861	4.27252, 4.18926
4th	6.9023	6.86841	6.36518	6.61803, 6.53875
5th	6.99999	8.83809	8.61754	8.76432, 8.67103

**Table 2**

Time-average rates of the functional convergence for the dual inconsistent discretization.

Accuracy	Advection	Heat	Burger's	System ( $J(p), J(u)$ )
3rd	3.06438	4.17441	3.93663	2.71162, 3.68422
4th	4.13107	5.22073	5.08856	3.41406, 3.72249
5th	4.64093	5.42542	5.60646	4.53447, 4.25429

**Table 3**Average errors using  $N = 32$  grid points.

Accuracy	Solution for $p$			Functional for $p$		
	Consistent	Wide	Compact	Consistent	Wide	Compact
3rd	2.0446e-03	2.0571e-03	1.6012e-03	5.0140e-05	2.8720e-04	5.6833e-04
4th	1.8328e-03	1.3131e-03	1.2423e-03	2.3244e-05	4.0409e-04	8.4830e-04
5th	1.1855e-02	6.9236e-03	6.9241e-03	1.2150e-05	1.2854e-03	3.1519e-03
	Solution for $u$			Functional for $u$		
	Consistent	Wide	Compact	Consistent	Wide	Compact
3rd	5.0395e-03	1.0337e-03	4.2541e-04	1.0125e-04	5.1268e-04	4.6830e-04
4th	2.1250e-03	1.0265e-03	4.1681e-04	1.6691e-05	3.1254e-04	3.6392e-04
5th	1.5030e-02	1.1059e-02	3.9369e-03	9.7499e-06	6.1595e-04	5.2289e-03

We stress that the method presented does not require any knowledge about the solution of the adjoint equations. Spatial dual consistency is a property of the discretization based upon knowledge of the form of the adjoint equation and its boundary conditions. Superconvergent functionals are thus obtained at no extra computational cost.

The superconvergence of the functional ensures that for sufficiently high resolutions, the dual consistent discretization will outperform a spatially dual inconsistent discretization. Most realistic simulations are, however, marginally or under-resolved and it is desirable that the higher order accuracy does not come at the cost of large error constants which ruin computations on a coarse mesh.

The errors in the solution and in the linear functionals were computed for a coarse mesh. The solution and functional errors were computed as a function of time for the coarsest grid level,  $N = 32$  grid points. We consider only the incompletely parabolic case to reduce the number of tables. The results were verified to be analogous for the other cases. We have also included an inconsistent scheme with a more accurate compact discretization of the second derivative as described in [20,52]. The errors are summarized in Table 3, where we present the average error over time for both the solutions and the functionals. From Table 3, we can see that the dual consistent discretization is somewhat less accurate in computing the solution, but much more accurate in computing the functionals. The 5th-order accurate spatially dual consistent discretization is already at 32 gridpoints 2 orders of magnitude more accurate than the spatially dual inconsistent discretization.

## 6. Summary and conclusions

We have defined and derived spatially dual consistent discretizations based on finite difference operators satisfying the summation-by-parts properties. The boundary conditions were imposed weakly using the simultaneous approximation term. We have presented derivations of spatial dual consistency in a general way and applied the technique to four representative equations; the advection equation, the heat equation, the viscous Burgers' equation and an incompletely parabolic system of equations.

In the cases we considered, the requirements for spatial dual consistency conform with the stability requirements. It was hence always possible to derive schemes which are both energy stable and spatially dual consistent for the cases we have considered, despite all model problems being of different type.

It was shown for all considered cases that a spatial dual consistent discretization produced superconvergent linear functionals computed from the solution. By superconvergence we mean that the solution is accurate of order  $p + 1$  (or  $p + 2$  under certain conditions), while the linear functional is computed with  $2p$ -order accuracy.

We have computed the errors in both the solution and in the linear functionals for a coarse mesh to ensure that the superconvergence does not come at the cost of large error constants. It was seen that the solution computed from the spatially dual consistent scheme was somewhat less accurate, while the functional could be two orders of magnitude more accurate already on a coarse grid.

The superconvergence does not require any knowledge about the solution of the adjoint equations. By considering only the form of the adjoint equation and its boundary conditions, it is a matter of choosing the SAT such that the scheme becomes stable and spatial dual consistent. Superconvergent functional outputs can thus be computed at no extra computational cost compared to a standard discretization.

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## References

- [1] Michael B. Giles, Niles A. Pierce, Adjoint equations in CFD: duality, boundary conditions and solution behaviour. In AIAA Paper 97-1850, 1997.
- [2] Michael B. Giles, Mats G. Larson, J. Mårten Levenstam, Endre Süli, Adaptive error control for finite element approximations of the lift and drag coefficients in viscous flow. Technical report, Report NA-97/06, Oxford University Computing Laboratory, 1997.
- [3] Niles A. Pierce, Michael B. Giles, Adjoint recovery of superconvergent functionals from PDE approximations, *SIAM Review* 42 (2) (2000) 247–264.
- [4] Michael B. Giles, Niles A. Pierce, Superconvergent lift estimates through adjoint error analysis. *Innovative Methods for Numerical Solutions of Partial Differential Equations*, 2001.
- [5] Niles A. Pierce, Michael B. Giles, Adjoint and defect error bounding and correction for functional estimates, *Journal of Computational Physics* 200 (November 2004) 769–794.
- [6] Michael B. Giles and Niles A. Pierce, On the properties of solutions of the adjoint Euler equations. *Numerical Methods for Fluid Dynamics VI ICFD*, pages 1–16, 1998.
- [7] Yingda Cheng, Chi-Wang Shu, Superconvergence of discontinuous galerkin and local discontinuous galerkin schemes for linear hyperbolic and convection-diffusion equations in one space dimension, *SIAM Journal on Numerical Analysis* 47 (6) (2010) 4044–4072.
- [8] Krzysztof J. Fidkowski, Output error estimation strategies for discontinuous galerkin discretizations of unsteady convection-dominated flows, *International Journal for Numerical Methods in Engineering* 88 (12) (2011) 1297–1322.
- [9] James Lu, A posteriori error control framework for adaptive precision optimization using discontinuous Galerkin finite element method. PhD thesis, Johann Radon Institute for Computational and Applied Mathematics, Austrian Academy of Sciences, 2005.
- [10] Todd A. Oliver, David L. Darmofal, Analysis of dual consistency for discontinuous galerkin discretizations of source terms, *SIAM Journal on Numerical Analysis* 47 (5) (2009) 3507–3525.
- [11] Karthik Mani, Dimitri J. Mavriplis, Error estimation and adaptation for functional outputs in time-dependent flow problems, *Journal of Computational Physics* 229 (January 2010) 415–440.
- [12] Kui Ou and Antony Jameson, Unsteady adjoint method for the optimal control of advection and Burgers' equations using high order spectral difference method. In 49th AIAA Aerospace Sciences Meeting, 2011.
- [13] Krzysztof J. Fidkowski, David L. Darmofal, Review of output-based error estimation and mesh adaptation in computational fluid dynamics, *AIAA Journal* 49 (4) (2011) 673–694.
- [14] Michael B. Giles, Endre Süli, Adjoint methods for PDEs: a posteriori error analysis and postprocessing by duality, *Acta Numerica* 11 (2002) 145–236.
- [15] Antony Jameson, Aerodynamic design via control theory, *Journal of Scientific Computing* 3 (September 1988) 233–260.
- [16] Michael B. Giles, Niles A. Pierce, An introduction to the adjoint approach to design, *Flow, Turbulence and Combustion* 65 (2000) 393–415.
- [17] Jason E. Hicken, David W. Zingg, Superconvergent functional estimates from summation-by-parts finite-difference discretizations, *SIAM Journal on Scientific Computing* 33 (2) (2011) 893–922.
- [18] Jason E. Hicken, Output error estimation for summation-by-parts finite-difference schemes, *Journal of Computational Physics* 231 (9) (2012) 3828–3848.
- [19] Bo Strand, Summation by parts for finite difference approximations for  $d/dx$ , *Journal of Computational Physics* 110 (1) (1994) 47–67.
- [20] Ken Mattsson, Jan Nordström, Summation by parts operators for finite difference approximations of second derivatives, *Journal of Computational Physics* 199 (2) (2004) 503–540.
- [21] Mark H. Carpenter, David Gottlieb, Saul Abarbanel, Time-stable boundary conditions for finite-difference schemes solving hyperbolic systems: Methodology and application to high-order compact schemes, *Journal of Computational Physics* 111 (2) (1994) 220–236.
- [22] M. Berndt, K. Lipnikov, M. Shashkov, M.F. Wheeler, I. Yotov, Superconvergence of the velocity in mimetic finite difference methods on quadrilaterals, *SIAM Journal on Numerical Analysis* 43 (4) (2005) 1728–1749.
- [23] Qiqi Wang, Parviz Moin, Gianluca Iaccarino, Minimal repetition dynamic checkpointing algorithm for unsteady adjoint calculation, *SIAM Journal on Scientific Computing* 31 (4) (2009) 2549–2567.
- [24] Steven M. Kast, Krzysztof J. Fidkowski, and Philip L. Roe, An unsteady entropy adjoint approach for adaptive solution of the shallow-water equations. In AIAA Paper Number 2011-3694, 2011.
- [25] Qiqi Wang, David Gleich, Amin Saberi, Nasrollah Etemadi, Parviz Moin, A monte carlo method for solving unsteady adjoint equations, *Journal of Computational Physics* 227 (12) (2008) 6184–6205.
- [26] Nail K. Yamaleev, Boris Diskin, Eric J. Nielsen, Local-in-time adjoint-based method for design optimization of unsteady flows, *Journal of Computational Physics* 229 (July 2010) 5394–5407.
- [27] Shengtai Li, Linda Petzold, Adjoint sensitivity analysis for time-dependent partial differential equations with adaptive mesh refinement, *Journal of Computational Physics* 198 (1) (2004) 310–325.
- [28] Heinz-Otto Kreiss and Godela Scherer, Finite element and finite difference methods for hyperbolic partial differential equations. In *Mathematical Aspects of Finite Elements in Partial Differential Equations*, number 33 in Publ. Math. Res. Center Univ. Wisconsin, pages 195–212. Academic Press, 1974.
- [29] Heinz-Otto Kreiss and Godela Scherer, On the existence of energy estimates for difference approximations for hyperbolic systems. Technical report, Uppsala University, Division of Scientific Computing, 1977.
- [30] Mark H. Carpenter, Jan Nordström, David Gottlieb, Revisiting and extending interface penalties for multi-domain summation-by-parts operators, *Journal of Scientific Computing* 45 (1–3) (2010) 118–150.
- [31] Jan Nordström, Jing Gong, Edwin van der Weide, Magnus Svärd, A stable and conservative high order multi-block method for the compressible Navier-Stokes equations, *Journal of Computational Physics* 228 (24) (2009) 9020–9035.
- [32] Magnus Svärd, Jan Nordström, On the order of accuracy for difference approximations of initial-boundary value problems, *Journal of Computational Physics* 218 (1) (2006) 333–352.
- [33] Ken Mattsson, Magnus Svärd, Mark Carpenter, Jan Nordström, High-order accurate computations for unsteady aerodynamics, *Computers and Fluids* 36 (3) (2007) 636–649.
- [34] Magnus Svärd, Jan Nordström, A stable high-order finite difference scheme for the compressible Navier-Stokes equations: No-slip wall boundary conditions, *Journal of Computational Physics* 227 (10) (2008) 4805–4824.
- [35] Magnus Svärd, Ken Mattsson, Jan Nordström, Steady-state computations using summation-by-parts operators, *Journal of Scientific Computing* 24 (1) (2005) 79–95.
- [36] X. Huan, Jason E. Hicken, and David W. Zingg, Interface and boundary schemes for high-order methods. In the 39th AIAA Fluid Dynamics Conference, AIAA Paper No. 2009-3658, San Antonio, USA, 22–25 June 2009.

- [37] Ken Mattsson, Magnus Svärd, Mohammad Shoeybi, Stable and accurate schemes for the compressible Navier-Stokes equations, *Journal of Computational Physics* 227 (February 2008) 2293–2316.
- [38] Pelle Olsson, Summation by parts, projections, and stability, I. *Mathematics of Computation* 64 (211) (1995) 1035–1065.
- [39] Pelle Olsson, Summation by parts, projections, and stability, II. *Mathematics of Computation* 64 (212) (1995) 1473–1493.
- [40] Jan Nordström, Mark H. Carpenter, High-order finite difference methods, multidimensional linear problems, and curvilinear coordinates, *Journal of Computational Physics* 173 (1) (2001) 149–174.
- [41] Jan Nordström, Conservative finite difference formulations, variable coefficients, energy estimates and artificial dissipation, *Journal of Scientific Computing* 29 (2006) 375–404.
- [42] Jeremy E. Kozdon, Eric M. Dunham, and Jan Nordström. Simulation of Dynamic Earthquake Ruptures in Complex Geometries Using High-Order Finite Difference Methods. Technical Report LiTH-MAT-R, 2012:2, Linköping University, Department of Mathematics, Sweden, 2011.
- [43] Ken Mattsson. Summation by parts operators for finite difference approximations of second-derivatives with variable coefficients. *Journal of Scientific Computing*, pages 1–33, 2011.
- [44] Jan Nordström, Magnus Svärd, Well-posed boundary conditions for the Navier–Stokes equations, *SIAM Journal on Numerical Analysis* 43 (3) (2005) 1231–1255.
- [45] Bertil Gustafsson, Heinz-Otto Kreiss, and Joseph Olinger. *Time Dependent Problems and Difference Methods*. Wiley Interscience, 1995.
- [46] Jason E. Hicken and David W. Zingg. Summation-by-parts operators and high-order quadrature. ArXiv e-prints, March 2011.
- [47] Bernardo Cockburn, Chi-Wang Shu, The local discontinuous galerkin method for time-dependent convection-diffusion systems, *SIAM Journal on Numerical Analysis* 35 (October 1998) 2440–2463.
- [48] Jing Gong, Jan Nordström, Interface procedures for finite difference approximations of the advection-diffusion equation, *Journal of Computational and Applied Mathematics* 236 (5) (2011) 602–620.
- [49] Heinz-Otto Kreiss and Jens Lorenz. *Initial-Boundary Value Problems and the Navier-Stokes Equations*. SIAM, 2004.
- [50] Saul Abarbanel, David Gottlieb, Optimal time splitting for two- and three-dimensional Navier-Stokes equations with mixed derivatives, *Journal of Computational Physics* 41 (1) (1981) 1–33.
- [51] Jens Lindström, Jan Nordström, A stable and high-order accurate conjugate heat transfer problem, *Journal of Computational Physics* 229 (14) (2010) 5440–5456.
- [52] Mark H. Carpenter, Jan Nordström, David Gottlieb, A stable and conservative interface treatment of arbitrary spatial accuracy, *Journal of Computational Physics* 148 (2) (1999) 341–365.