Derive boundary conditions for holistic discretisations of Burgers’ equation

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Abstract

I previously used Burgers’ equation to introduce a new method of numerical discretisation of PDEs. The analysis is based upon centre manifold theory so we are assured that the discretisation accurately models all the processes and their subgrid scale interactions. Here I show how boundaries to the physical domain may be naturally incorporated into the numerical modelling of Burgers’ equation. We investigate Neumann and Dirichlet boundary conditions. As well as modelling the nonlinear advection, the method naturally derives symmetric matrices with constant bandwidth to correspond to the self-adjoint diffusion operator. The techniques developed here may be used to accurately model the nonlinear evolution of quite general spatio-temporal dynamical systems on bounded domains.

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1 Introduction

We discuss the holistic discretisation of boundary conditions for partial differential equations. Holistic discretisation is based upon the support centre manifold theory gives to the nonlinear dynamics on finite grid spacing. We expect such discretisation will have good stability and high accuracy on coarse grids because it systematically accounts for subgrid scale interactions. To date we have considered periodic problems and their initial conditions. Here we show how to incorporate different boundary conditions into the analysis.

As an illustrative example we restrict attention to the one-dimensional spatial discretisation of Burgers’ equation

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial x^2}, \tag{1} \]

which contains the important mechanisms of diffusion and nonlinear advection. As example boundary conditions we consider the important cases of Dirichlet, and Neumann boundary conditions. The same techniques may be easily extended to other partial differential equations, other boundary conditions and higher spatial dimensions.

The centre manifold analysis is based upon dividing the domain into finite sized elements, each separated from their two neighbours by specially crafted artificial internal boundary conditions (IBCs). The form of the IBCs generates a discretisation in the interior of the domain which is not only linearly consistent, as proved in, but which appears to be nonlinearly consistent to high order. This observation is based upon this analysis of Burgers’ equation and work in progress on the Kuramoto-Sivashinsky equation; further research is needed to prove it in general.

But the focus here is on the discretisation near the boundary of the domain. Boundary conditions are easily incorporated simply by replacing an IBC of an end element by a variant of the actual boundary condition: the Dirichlet boundary condition of fixed field is implemented as; the Neumann boundary condition of fixed flux is. The computer algebra
Holistic discretisation of Burgers’ equation in the interior

We consider Burgers’ equation (1) on some finite domain in $x$. Place grid points $x_j$ equi-spaced across the domain with constant spacing $h$, and correspondingly define $u_j = u(x_j, t)$, that is, $u_j$ is the evolving field $u$ evaluated at the $j$th grid point. Divide the domain into $m$ elements with a grid point at the centre of each. Following [5] to apply centre manifold theory we distinguish each element using internal boundary conditions (IBCs) in the discrete form

$$ \mu_x \delta_x v_j(x, t) = \gamma \mu \delta u_j \quad \text{and} \quad \delta^2_x v_j(x, t) = \gamma \delta^2 u_j, $$

(2)
evaluated at $x = x_j$ where $v_j$ denotes the field in the $j$th element. As shown in [6], this particular choice of IBCs ensures that the resultant finite difference scheme is consistent to high order in $h$ as the grid size $h \to 0$. In this section we repeat the construction of the holistic discretisation, following [6], away from the domain boundaries via centre manifold theory but with a new and convenient form of these discrete IBCs.

In actually developing finite difference models the IBCs may take any of many equivalent forms [6, e.g.]. In later sections we investigate the discretisation near a boundary of the domain: the element adjacent a boundary has...
one real boundary and one artificial internal boundary. Thus it is appropriate to rewrite the two IBCs in (2) in the form of two conditions, one at the left edge of each internal element, and one at the right. Recall that the difference operators $\mu \pm \frac{1}{2} \delta = E^{\pm 1/2}$ \text{[3, p65, e.g.]} so that to the first IBC in (2) add/subtract half the second to give the equivalent IBCs

\[ \delta_x v_j(x, t) = \gamma \delta u_{j-1/2} \quad \text{at} \quad x = x_{j-1/2}, \quad (3) \]
and
\[ \delta_x v_j(x, t) = \gamma \delta u_{j+1/2} \quad \text{at} \quad x = x_{j+1/2}. \quad (4) \]

The IBC (4) is to hold at the right-hand side of each element and the IBC (3) is to hold at the left. The introduced parameter $\gamma$, when non-zero, couples each element to its neighbour. When $\gamma = 0$ these IBCs effectively insulate each element from its neighbours and forms the basis of the centre manifold analysis; whereas when $\gamma = 1$ they assert that the field in the $j$th element when extended into the surrounding elements has the same differences centred across each internal boundary as that given by the grid point values. Thus evaluating the model at $\gamma = 1$ forms the relevant discretisation. These IBCs apply to all elements except for the leftmost and rightmost elements, the ones adjacent to the boundary: in the leftmost element the left-hand IBC, (3) with $j = 1$, is replaced by the actual boundary condition; in the rightmost element the right-hand IBC, (4) with $j = m$, is replaced by the actual boundary condition. In this paper I analyse the left boundary of the domain—discretisations near the right boundary are similar by symmetry.

In the interior of the domain the boundaries of the domain have no influence upon the discretisation. Each element in the interior has IBCs (3) and (4). Executing the computer algebra program in Appendix A, adapted from \text{[3]}, the subgrid structure of the solution field $u(x, t)$ is, in terms of $\xi = (x - x_j)/h$,

\[ v_j = u_j + \gamma \left[ \xi \mu \delta u_j + \frac{1}{2} \xi^2 \delta^2 u_j \right] + \gamma^2 \left[ \frac{1}{6} (\xi^3 - \xi) \mu \delta^3 u_j + \frac{1}{24} (\xi^4 - \xi^2) \delta^4 u_j \right] \\
+ \gamma h \left[ \frac{1}{6} (\xi^3 - \xi) u_j \delta^2 u_j + \mathcal{O}(\|u\|^3 + \gamma^3) \right]. \quad (5) \]

The corresponding evolution on this centre manifold forms the holistic discretisation in the interior:

\[ \dot{u}_j = \frac{1}{h^2} \left[ \gamma \delta^2 u_j - \frac{\gamma^2}{12} \delta^4 u_j + \frac{\gamma^3}{90} \delta^6 u_j \right] \\
- \frac{1}{h} u_j \left[ \gamma \mu \delta u_j - \frac{\gamma^2}{6} \mu \delta^3 u_j \right] + \frac{\gamma^2}{24 h} \left( \delta^2 u_j \mu \delta u_j + \delta^4 u_j \mu \delta^3 u_j \right) \\
+ \frac{\gamma}{12} u_j^2 \delta^2 u_j + \mathcal{O}(\|u\|^4 + \gamma^4). \quad (6) \]
As discussed previously \cite{6} when the coupling parameter \( \gamma = 1 \): the first line gives successive approximations to the diffusion term \( u_{xx} \); the second line gives approximations to the nonlinear advection; and lastly, the cubic nonlinear term, \( u^2_2 \delta^2 u_j \) in the last line above, accounts for subgrid scale interactions between the advection and diffusion and acts to stabilise the numerical model. Higher-order terms are easily found by the computer algebra of Appendix A but for clarity are not presented here. In the limit as the grid spacing \( h \to 0 \) higher-order discretisations have the equivalent pde

\[
\frac{\partial u}{\partial t} = \gamma \left[ -u \frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2} \right] + \frac{h^2}{12} (1 - \gamma) \left[ u_{xxxx} - 2u u_{xxx} + u^2 u_{xx} \right]
\]

\[
+ \frac{h^4}{720} (1 - \gamma) \left[ 2\gamma (-5u^2_x u_{xx} - 9uu^2_{xx} - 25uu_x u_{xxx} + 15u_x u_{xxxx}) + 15u_x u_{xxxx} - 2u^2 u_{xxxx} \right] + (1 - 4\gamma)(2\partial^6_x u - 6u\partial^5_x u + 5u^2 \partial^4_x u) \right]
\]

\[+ \mathcal{O}(\|u\|, \gamma^4, h^6). \tag{7} \]

(2)

See that upon substituting \( \gamma = 1 \) to recover a discretisation for the Burgers’ equation (1), we would find an equivalent pde to an error \( \mathcal{O}(h^6, \|u\|^4) \). Analogous lower order discretisations are obtained, as promised by the analysis in \cite{5}, when we truncate the discretisation (3) to lower orders in the coupling parameter \( \gamma \). But observe the new feature that the discrete form (3–4) of the ibcs lead to discretisations which are not only linearly consistent, as assured in \cite{5}, but are also nonlinearly consistent. Further research is needed to establish nonlinear consistency in general.

### 3 Dirichlet boundary conditions applied at a grid point

Consider the case of Dirichlet conditions on the boundary of the domain of prescribed \( u \) at a grid point; without loss of generality say

\[ u = a(t) \text{ at } x = x_0. \tag{8} \]

This boundary condition is included in the analysis simply by replacing the left-hand ibc in the leftmost element, (3) with \( j = 1 \), by (as if \( u_0 = a \) in (3))

\[ \delta_x v_1(x, t) = \gamma (u_1 - a) \text{ at } x = x_{1/2}. \tag{9} \]

(Implicitly the first element then extends from \( x_0 = x_1 - h \) to \( x_1 + h/2 \).) When the coupling parameter \( \gamma = 0 \) this ibc effectively insulates the first
element from the conditions at the domain boundary. However, when \( \gamma = 1 \), since \( v_j(x_j, t) = u_j \), this reduces to (8) by requiring \( v_1(x_0, t) = a \). Hence, the centre manifold derivation is based on \( \gamma = 0 \) as explained in [6] and evaluated at \( \gamma = 1 \) to obtain a discretisation of Burgers’ equation.

We then solve for the subgrid fields in the elements near the boundary, \( j = 1, 2, \ldots \). The computer algebra program in Appendix A implements this boundary condition when \texttt{dirichlet:=1}. The influence of this specified boundary value affects a number of elements near the boundary equal to the order of \( \gamma \) retained in the analysis, nothing else: in the interior the discretisation is (8); whereas for elements the near the boundary and for errors \( O(\|u\|^4 + \gamma^4) \) we find the evolution to be of the form

\[
\begin{bmatrix}
\dot{u}_1 \\
\dot{u}_2 \\
\dot{u}_3
\end{bmatrix} = \frac{1}{h^2}(Du + f_d) - \frac{1}{h}(UCu + g_c(u) + f_c) + (U^2Bu + f_b) + O(\|u\|^4 + \gamma^4),
\]

where \( U = \text{diag}(u_1, u_2, u_3) \) is the diagonal matrix of grid velocities and the three parts of the right-hand side represent respectively the discretisation of the diffusion, the nonlinear advection, and the leading order interaction between advection and diffusion. These parts include the forcing due to the time dependent boundary value \( a \). Here the various terms are found to be:

\[
D = \gamma \begin{bmatrix}
-2 & 1 & 1 & \cdots \\
1 & -2 & 1 & \cdots \\
1 & -2 & 1 & \cdots \\
\end{bmatrix} - \frac{\gamma^2}{12} \begin{bmatrix}
5 & -4 & 1 & \cdots \\
-4 & 6 & -4 & 1 & \cdots \\
1 & -4 & 6 & -4 & 1 \end{bmatrix} + \frac{\gamma^3}{90} \begin{bmatrix}
-14 & 14 & -6 & 1 & \cdots \\
14 & -20 & 15 & -6 & 1 & \cdots \\
-6 & 15 & -20 & 15 & -6 & 1 \end{bmatrix} + O(\gamma^4) \tag{11}
\]

\[
C = \frac{\gamma}{2} \begin{bmatrix}
0 & 1 & \cdots \\
-1 & 0 & 1 & \cdots \\
 & -1 & 0 & 1 \\
\end{bmatrix} - \frac{\gamma^2}{12} \begin{bmatrix}
0 & -2 & 1 & \cdots \\
2 & 0 & -2 & 1 & \cdots \\
-1 & 2 & 0 & -2 & 1 \\
\end{bmatrix} + O(\gamma^3) \tag{12}
\]

\[
g_c = \frac{\gamma^2}{24} \begin{bmatrix}
\frac{1}{2} u^T G_1 u \\
\frac{1}{2} u^T G_2 u \\
\frac{1}{2} u^T G_3 u
\end{bmatrix} \quad \text{where} \quad G_1 = \begin{bmatrix}
2 & 5 & -1 \\
5 & -6 & 1 \\
-1 & 1 & 0
\end{bmatrix}, \quad G_2 = \begin{bmatrix}
6 & -5 & 0 & 0 \\
-5 & 0 & 5 & -1 \\
0 & 5 & -6 & 1 \\
0 & -1 & 1 & 0
\end{bmatrix}, \quad G_3 = \begin{bmatrix}
0 & -1 & 1 & 0 & 0 \\
-1 & 6 & -5 & 0 & 0 \\
1 & 5 & 0 & 5 & -1 \\
0 & 0 & 5 & -6 & 1 \\
0 & 0 & -1 & 1 & 0
\end{bmatrix}. \tag{13}
\]
and $B = \frac{1}{12}D + \mathcal{O}(\gamma)$. Denote by $\mathcal{D}$ the matrix appearing above in $D$ linear in $\gamma$ and then row extended across the interior of the domain: $\mathcal{D}$ is the matrix of the second-order centred approximation to the second derivative, $\delta^2$. Observe that the order $\gamma^2$ and $\gamma^3$ matrices in $D$ simply correspond to $\mathcal{D}^2$ and $\mathcal{D}^3$. Thus the discretisation of the diffusion term, across the entire domain including the near boundary elements, is simply $\gamma\delta^2 - \frac{\gamma^2}{12}\delta^4 + \frac{\gamma^3}{90}\delta^6$ seen in the first line of the interior discretisation, (3), but with the matrix $\mathcal{D}$ replacing the centred difference $\delta^2$. Thus this approach generates an appropriately symmetric discretisation of the self-adjoint diffusion term $u_{xx}$. The nonlinear stabilisation term, $U^2Bu$, also corresponds to replacing $\delta^2$ in (3) by $\mathcal{D}$. Similarly, denote by $\mathcal{C}$ the matrix appearing above in $C$ linear in $\gamma$ (including the factor $\frac{1}{2}$) and then row extended across the interior of the domain: $\mathcal{C}$ is the matrix of the second-order centred approximation to the first derivative, $\mu\delta$. Observe that the order $\gamma^2$ matrix in $\mathcal{C}$ is $(\mathcal{DC} + \mathcal{CD})/2$ corresponding to the average of different permutations of the centred difference operators $\mu\delta^3$. Thus again the discretisation of the advection terms across the entire domain is the interior discretisation, $\gamma\mu\delta - \frac{\gamma^2}{6}(\mu\delta\delta^2 + \delta^2\mu\delta)/2$, with the truncated $\mathcal{C}$ and $\mathcal{D}$ replacing the difference operators $\mu\delta$ and $\delta^2$ respectively. Additional terms represented by $g_c$ for the discretisation of the advection correspond to the nonlinear higher order term $\frac{\gamma^2}{24h}(\delta^2u_j \mu\delta^3u_j + \delta^4u_j \mu\delta^3u_j)$ in the model (3). These are pleasing patterns.

Also see that by truncating to a fixed power of the inter-element coupling parameter $\gamma$ we will obtain a discretisation that has constant bandwidth across the whole domain. This constant bandwidth will always be derived in this holistic approach, see for another example the Neumann boundary conditions in the next section, because the truncation at a fixed power of the inter-element coupling $\gamma$ controls how many neighbouring elements interact with any given element. Although there is a lower order (in $h$) of consistency near the domain boundaries, the support by centre manifold theory is the same across the whole domain. As discussed in [3], the reason for this support is that the theory applies to the solutions of Burgers’ PDE (1) in the entire domain, not just in some locale.

Now consider the forcing from the boundary. Using $a = (a, h^2\dot{a})$, it is

$$
\begin{align*}
f_d &= \left[ \begin{array}{ccc}
\gamma + \frac{\gamma^2}{6} + \frac{\gamma^3}{18} & -\frac{\gamma}{12} - \frac{\gamma^2}{45} - \frac{\gamma^3}{112} \\
-\frac{\gamma^2}{12} & -\frac{2\gamma^3}{45} & \frac{\gamma^2}{90} + \frac{\gamma^3}{140} \\
\frac{\gamma^2}{90} & \frac{\gamma^3}{560}
\end{array} \right] a + \mathcal{O}(\gamma^4, \dot{a}),
\end{align*}
\quad (14)
$$
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\[ f_c = \gamma \begin{bmatrix} \frac{1}{2} u_1 & -\frac{1}{24} u_1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} a + \frac{\gamma^2}{24} \begin{bmatrix} 4u_1 + 3a & \frac{1}{15}(7u_1 - 2u_2 - 9a) + \frac{5}{168} h^2 \dot{a} \\ -(u_1 + u_2) & \frac{2}{15} (u_1 + u_2) \\ 0 & 0 \end{bmatrix} a + \mathcal{O}(\gamma^3, \ddot{a}), \]  

(15)

\[ f_b = \frac{\gamma}{12} \begin{bmatrix} u_1^2 & -\frac{1}{15} u_1^2 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} a + \mathcal{O}(\gamma^2, \ddot{a}). \]  

(16)

See that this holistic approach not only involves the value \( a \) of the field at the boundary in the diffusion term, it also involves \( a \) in the nonlinear advection (in \( f_c \)) and in the nonlinear stabilisation (in \( f_b \)). But further, it also involves time derivatives of the boundary value \( a \). The reason is clearly that changes in \( a \) take time to advect and diffuse into the interior of the first few elements and so the effect of changes in the boundary value \( a \) upon the evolution of the grid values will lag, as seen by the opposite sign of the coefficients in the two columns of (14). This lag increases with the element size \( h \) and hence accounts for the \( h^2 \) factor multiplying every \( \dot{a} \). Similarly, though not recorded above, higher order analysis shows each second derivative appears only in the combination \( h^4 \ddot{a} \). Such effects are important when we try to use, in large scale problems, the expected accuracy and stability of these holistic discretisations on coarse grids.

4 Apply Neumann boundary conditions at a midpoint

Consider PDEs with Neumann boundary conditions of prescribed gradient of the field \( u \). Two different sorts of numerical approximations are commonly developed for such a boundary condition: a grid point is placed at the boundary (as for the Dirichlet problem of §3); or the boundary is arranged to be midway between two grid points. For the first case I found that the discretisation of the diffusion is expressed in terms of non-symmetric matrices. For the second case, the matrices are symmetric which again corresponds to the self-adjoint nature of the diffusion operator. Thus I report here on the second case where the boundary is at a midpoint of the grid.

Without loss of generality, let the Neumann boundary condition of pre-
Apply Neumann boundary conditions at a midpoint be
\[
\hat{h} \frac{\partial u}{\partial x} = \gamma a(t) \quad \text{at } x = x_{1/2},
\]  
(17)

where, as for the IBCs, we actually are interested in the case \( \gamma = 1 \). To supplement this left-hand boundary condition on the leftmost element we use the IBC (4) as before. We execute the computer algebra program of Appendix A with options \texttt{dirichlet:=0} and \texttt{midpoint:=1}. Again the interior discretisation is (6) whereas in elements the near the boundary we find the grid values evolve according to the form (10) where now the matrices are

\[
\mathcal{D} = \gamma \begin{bmatrix}
-1 & 1 & -2 & 1 & \cdots \\
1 & -2 & 1 & & \\
1 & -2 & 1 & & \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
\end{bmatrix} - \frac{\gamma^2}{12} \begin{bmatrix}
2 & -3 & 1 & \cdots \\
-3 & 6 & -4 & 1 & \\
1 & -4 & 6 & -4 & 1 \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
\end{bmatrix} + \mathcal{O}(\gamma^4),
\]
\[
\mathcal{C} = \frac{\gamma}{2} \begin{bmatrix}
-1 & 1 & 0 & 1 & \cdots \\
1 & -2 & 1 & & \\
-1 & 0 & 1 & & \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
\end{bmatrix} - \frac{\gamma^2}{12} \begin{bmatrix}
1 & -2 & 1 & \cdots \\
1 & 0 & -2 & 1 & \\
-1 & 2 & 0 & -2 & 1 \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
& & & & \\
\end{bmatrix} + \mathcal{O}(\gamma^3),
\]
\[
g_c = \frac{\gamma}{24} \begin{bmatrix}
-u_1^2 + u_2^2 \\
0 \\
0 \\
\end{bmatrix} + \frac{\gamma^2}{24} \begin{bmatrix}
\frac{1}{2} u^T G_1 u \\
\frac{1}{2} u^T G_2 u \\
\frac{1}{2} u^T G_3 u \\
\end{bmatrix}
\]

where

\[
G_1 = \begin{bmatrix}
-\frac{49}{12} & \frac{19}{4} & \frac{15}{4} & \\
\frac{19}{4} & \frac{15}{4} & \frac{11}{4} & \\
\frac{15}{4} & \frac{11}{4} & \frac{19}{4} & \\
\end{bmatrix},
G_2 = \begin{bmatrix}
\frac{23}{6} & \frac{-47}{12} & 0 & 0 \\
\frac{-47}{12} & 0 & 5 & -1 \\
0 & 5 & -6 & 1 \\
0 & -1 & 1 & 0 \\
\end{bmatrix}
\]
\[
B = \frac{\gamma}{12} \hat{\mathcal{D}} + \frac{\gamma}{12} \begin{bmatrix}
-\frac{1}{18} & \frac{48}{18} & \frac{48}{18} & \cdots \\
0 & 0 & 0 & \\
0 & 0 & 0 & \\
\end{bmatrix} + \mathcal{O}(\gamma^2),
\]

(20)

and \( G_3 \) is as in (13). Denote by \( \hat{\mathcal{D}} \) the symmetric matrix appearing above in \( \mathcal{D} \) linear in \( \gamma \) and then row extended across the interior of the domain: \( \hat{\mathcal{D}} \) is

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1Neumann conditions at a grid point, say \( x_1 \), may be incorporated into the analysis by similarly requiring \( \hat{h} \partial u/\partial x = \gamma a \) at \( x = x_1 \) in place of the left-hand IBC (3).

2The computer algebra algorithm takes a few more iterations to complete because the algorithm is tuned to the discrete form of the IBC (3) whose left-hand side is only approximately that of (17).
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the matrix of the second-order centred approximation to the second derivative, \( \delta^2 \), but incorporating a zero derivative condition to the left of the grid. Observe in the order \( \gamma^2 \) and \( \gamma^3 \) matrices of \( \mathcal{D} \) that the discretisation near the boundary of the diffusion term, \( (18) \), is simply the interior discretisation seen in the first line of \( (6) \) with the truncated \( \tilde{\mathcal{D}} \) replacing the centred difference \( \delta^2 \).

Although here there is no clear pattern in \( \mathcal{C} \) nor \( \mathcal{B} \), as written above see that: \( \mathcal{B} \) is numerically close to \( \tilde{\mathcal{D}}/12 \); and, upon denoting \( \tilde{\mathcal{C}} \) as the matrix linear in \( \gamma \) in \( \mathcal{C} \), the \( \gamma^2 \) matrix is \( (\tilde{\mathcal{D}} \tilde{\mathcal{C}} + \tilde{\mathcal{C}} \tilde{\mathcal{D}})/2 \) just as for the Dirichlet boundary conditions. However, in this case the identification is a little forced because numerically small discrepancies have been gathered into \( \mathcal{C} \) along with indistinguishable similar terms corresponding to \( \gamma^2 (\delta^2 u_j \mu \delta^3 u_j + \delta^4 u_j \mu \delta u_j) \) appearing in the interior discretisation \( (6) \). Nonetheless the closeness of the match and the appropriate symmetry is reassuring.

The forcing from the boundary takes the form

\[
\begin{align*}
\mathbf{f}_d &= \begin{bmatrix}
-\gamma - \frac{\gamma^2}{12} - \frac{\gamma^3}{35} + \frac{\gamma}{24} + \frac{11\gamma^2}{1440} + \frac{\gamma^3}{378} \\
+ \frac{\gamma^2}{12} + \frac{\gamma^3}{30} & - \frac{11\gamma^2}{1440} - \frac{\gamma^3}{292} \\
- \frac{\gamma^3}{90} & \frac{\gamma^3}{700}
\end{bmatrix} \mathbf{a} + \mathcal{O}(\gamma^4, \ddot{\mathbf{a}}), \quad (22)
\end{align*}
\]

\[
\begin{align*}
\mathbf{f}_c &= \gamma \begin{bmatrix}
-\frac{11}{24} u_1 + \frac{31}{960} u_1 \\
0 & 0 \\
0 & 0
\end{bmatrix} \mathbf{a}
+ \frac{\gamma^2}{24} \begin{bmatrix}
-\frac{1}{6} u_1 - \frac{11}{60} u_2 - \frac{199}{120} a & \frac{224 u_1 - 577 u_2 - 3223 a}{53520} u_1 + \frac{11}{120} u_2 \\
- \frac{11}{12} a_1 + u_2 & \frac{199}{480} u_1 + \frac{11}{120} u_2
\end{bmatrix} \mathbf{a}
+ \mathcal{O}(\gamma^3, \ddot{\mathbf{a}}), \quad (23)
\end{align*}
\]

\[
\begin{align*}
\mathbf{f}_b &= \frac{\gamma}{12} \begin{bmatrix}
- \frac{49}{48} u_1^2 + \frac{657}{5760} u_1^2 \\
0 & 0 \\
0 & 0
\end{bmatrix} \mathbf{a} + \mathcal{O}(\gamma^2, \ddot{\mathbf{a}}). \quad (24)
\end{align*}
\]

As discussed in the previous section, the boundary value for the flux \( \mathbf{a} \) appears in a wide range of terms in the discretisation near the boundary. The reason again is that the flux feeds into the subgrid scale fields of the boundary elements and so affects the interaction between the various physical processes. The scope for such interaction increases with increasing element size \( h \) and so accounts for the appearance of the \( h^2 \) factor in front of the time derivative \( \ddot{\mathbf{a}} \). We need to know such effects on coarse grids.
5  Conclusion

We have considered the discretisation of Burgers’ equation (1) on a finite domain as a worked example of incorporating physical boundary conditions into the derivation of holistic discretisations. The two most common physical boundary conditions were considered in §3 and §4. Crucially we found: it is easy to maintain the symmetry appropriate to self-adjoint differential operators; discretisations are developed with constant bandwidth across the whole domain; and lastly our resolution of subgrid scale processes shows how time derivatives of the boundary forcing should also be included in the discretisation.

Additionally, using the discrete form of the inter-element boundary conditions (3–4) we observe for the first time a high order consistency of the nonlinear dynamics of Burgers’ equation.

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[5] A. J. Roberts. A holistic finite difference approach models linear dynamics consistently. Technical report, http://arXiv.org/abs/math.NA/0003135, March 2000.
Straightforward computer algebra programs are written to find the centre manifold and the evolution thereon [4, e.g.]. To ensure correctness and to provide a basis for further work I include the computer algebra code. This replaces extensive recording of elementary algebraic steps in the derivation of the results.

I implement the construction algorithm in REDUCE\(^3\). The overall plan of the algorithm is to iteratively satisfy Burgers’ equation (1) and the relevant internal (3–4) and actual boundary conditions. A general interior element is analysed in lines 47–53 while the \(o:=3\) elements near the boundary are analysed in the loop of lines 54–71. Although there are many details in the program, the correctness of the results are only determined by driving to zero (lines 53, 70 and 73) the residuals of Burgers’ equation in each element and the internal and domain boundary conditions: lines 47–9 evaluate the residuals for an arbitrary interior element; lines 55–8 for near domain boundary elements; and lines 60 or 62 the domain boundary condition. The other details, such as the updates computed in lines 50–2 and 67–9, only affect the rate of convergence to the ultimate answer.

[6] A. J. Roberts. Holistic discretisation ensures fidelity to Burgers’ equation. *Applied Numerical Modelling*, 37:371–396, 2001.

[7] A. J. Roberts. Holistic projection of initial conditions onto a finite difference approximation. Technical report, http://arXiv.org/abs/math.NA/0101205, 2001.
A Computer algebra derives different boundary discretisations

% improve printing
on div; off allfac; on revpri; factor gam,h;

% make function of \( \xi = (x - x_j)/h \)
depend xi,x;
let df(xi,x) => 1/h;

% solvability condition
operator solg; linear solg;
let { solg(xi^p,xi) => (1+(-1)^p)/(p+2)/(p+1)
  , solg(xi,xi) => 0, solg(1,xi) => 1 };%

% solves \( v'' = \text{RHS} \) s.t. \( v(0) = 0 \) and \( v(+1) = v(-1) \)
operator solv; linear solv;
let { solv(xi^p,xi) =>
  ( xi^(p+2)-(1-(-1)^p)*xi/2 )/(p+1)/(p+2)
  , solv(xi,xi) => (xi^3-xi)/6
  , solv(1,xi) => (xi^2)/2 };%

% parametrise with evolving \( u(j) \) and boundary forcing \( a \)
operator u; depend u,t;
let { df(u^k,t) => sub(j=k,gj)
  when (not fixp(k)) or (fixp(k) and k>0)
  , df(u^k,t) => g(k) when fixp(k) and k<=o and k>0 };%
operator a; depend a,t;

% linear solution in \( j \)th element
array g(o),v(o);
vj := u(j);
gj := 0;
for j:=1:o do v(j) := u(j);

% iterative refinement to specified error
% here work to error \( |u|^4 + \text{gam}^4 \) by multiplying advection by \text{gam}
let { \text{gam}^4 => 0, df(a,t,2) => 0 };%
repeat begin % first do interior elements
  deq := -df(vj,t) - \text{gam}*(u(j+1)-u(j)) + df(vj,x);
  rbc := -(sub(xi=+1,vj)-sub(xi=0,vj)) + \text{gam}*(u(j+1)-u(j));
  lbc := -(sub(xi=0,vj)-sub(xi=-1,vj)) + \text{gam}*(u(j)-u(j-1));
  gd := (rbc-lbc)/h^2 + solg(deq,xi);
  gj := gj + gd;
  vj := vj + h^2*solv(-deq+gd,xi) + xi*(rbc+lbc)/2;
A Computer algebra derives different boundary discretisations

```
ok:=if (deq=0) and (rbc=0) and (lbc=0) then 1 else 0;
for j:=1:o do begin % near boundary elements
    deq:=-df(v(j),t)-gam*v(j)*df(v(j),x)+df(v(j),x,2);
    rbc:=-(sub(xi=+1,v(j))-sub(xi=0,v(j)))+gam*(u(j+1)-u(j));
    if j>1 then % internal left BC
        lbc:=-sub(xi=0,v(j))+sub(xi=-1,v(j))+gam*(u(j)-u(j-1))
    else if dirichlet then % dirichlet at x_0
        lbc:=-sub(xi=0,v(1))+sub(xi=-1,v(1))+gam*(u(1)-a)
    else if midpoint then % neumann at x_1/2
        lbc:=-sub(xi=-1/2,h*df(v(1),x))+gam*a
    else begin % neumann at x_1
        abc:=-sub(xi=0,h*df(v(1),x))+gam*a;
        lbc:=2*abc-rbc;
    end;
    gd:=(rbc-lbc)/h^2+solg(deq,xi);
    g(j):=g(j)+gd;
    v(j):=v(j)+h^2*solv(-deq+gd,xi)+xi*(rbc+lbc)/2;
    ok:=if (deq=0) and (rbc=0) and (lbc=0) then ok else 0;
end;
showtime;
end until ok=1;
end;
```