Stability and Convergence Analysis of Fully Discrete Fourier Collocation Spectral Method for 3-D Viscous Burgers' Equation

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Abstract This paper analyzes the stability and convergence of the Fourier pseudospectral method coupled with a variety of specially designed time-stepping methods of up to fourth order, for the numerical solution of a three dimensional viscous Burgers' equation. There are three main features to this work. The first is a lemma which provides for an L^2 and H^1 bound on a nonlinear term of polynomial type, despite the presence of aliasing error. The second feature of this work is the development of stable time-stepping methods of up to fourth order for use with pseudospectral approximations of the three dimensional viscous Burgers' equation. Finally, the main result in this work is that the pseudospectral method coupled with the carefully designed time-discretizations is stable provided only that the time-step and spatial grid-size are bounded by two constants over a finite time. It is notable that this stability condition does not impose a restriction on the time-step that is dependent on the spatial grid size, a fact that is especially useful for three dimensional simulations.

Keywords 3-D viscous Burgers' equation · Fully discrete pseudospectral scheme · Aliasing error · Stability and convergence · A priori assumption · Multi-step schemes

1 Introduction

In this paper we consider the stability and convergence of the fully discrete approximation of the three-dimensional viscous Burgers' equation with periodic boundary conditions,

$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = \boldsymbol{v} \Delta \boldsymbol{u}, \tag{1}$$

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where $u = (u, v, w)^T$ is the velocity field in the *x*, *y*, and *z* directions, and v > 0 is the viscosity. On the partial differential equation (PDE) level, we know that the maximum principle (in time) is preserved for *u*, and a global in time smooth solution was proven in [25]. An alternate approach avoids the use of maximum principles; instead, the anti-symmetrization form of the nonlinear term is used to establish the well-posedness for (1) for all time. See the related discussions in [43] and numerical works [13, 15], etc.

In this work, we discretize the spatial terms using a Fourier collocation (pseudospectral) method, and the time-derivative using a variety of suitably chosen semi-implicit multistep methods. The notable result in this paper is that the stability analysis is performed on the collocation case, which is more difficult due to the presence of aliasing errors, and for the fully discrete case.

Spectral and pseudospectral methods were first studied in the 1970s, and are still analyzed today. There is a wide and varied literature on the spectral schemes. For linear time-dependent problems, the stability analysis typically relies on eigenvalue estimates [14, 24, 33]. For nonlinear problems, the theoretical foundation was laid in the pioneering works of Maday and Quarteroni [29–31] for steady-state spectral solutions. In the 1980s and 1990s there was significant growth in the field of spectral and pseudospectral methods for time-dependent nonlinear PDEs. In particular, we note the analysis of one-dimensional conservation laws by Tadmor and collaborators [9, 21, 28, 32, 39–42], semi-discrete viscous Burgers' equation and Navier-Stokes equations by E [44, 45], and the Galerkin spectral method for Navier-Stokes equations led by Guo [16, 17, 20, 21] and Shen [12, 18], among others.

However, the aforementioned theoretical developments in spectral and pseudospectral approximations to nonlinear time-dependent PDEs only considered the spatial approximation with the time variable kept continuous. Very few works have analyzed a fully discrete (discrete both in space and time) pseudospectral method applied to nonlinear problems. Among the existing ones, it is worth mentioning Bressan and Quarteroni's work [5] on the one-dimensional viscous Burgers' equation with a Cheyshev collocation differentiation in space. Their work relies on the 1-D structure of the solution and required a time step constraint of the form $\Delta t \leq Ch^{d/2}$ (with Δt the time-step, *h* the spatial grid size, and *d* the dimension) to ensure numerical stability. In that work, the authors remark that such a constraint is acceptable for a 1-D problem. However, it becomes a serious numerical challenge for multi-dimensional (especially for 3-D, d = 3) problems.

A careful analysis shows that such a time step constraint comes from an application of the inverse inequality to bound the L^{∞} norm of the numerical solution in terms of the L^2 norm: $||f||_{\infty} \leq Ch^{-d/2} ||f||_2$, for the numerical error function. It is well-known that an L^{∞} bound of the numerical solution is crucial in the establishment of stability and convergence for a fully discrete scheme applied to nonlinear PDEs. In fact, a time step constraint of this type is usually required when the inverse inequality is used in the nonlinear analysis. Some examples of this can be seen in the works [1, 11] for KDV type equations (with a constraint $\Delta t \leq Ch^2$) and [19] for a Galerkin spectral method for Navier-Stokes equations (with $\Delta t \leq Ch^{d/2}$).

In this work we provide a novel stability and convergence analysis for the Fourier collocation (pseudospectral) method, coupled with a number of carefully tailored time discretizations for the three dimensional viscous Burgers' equation. We design stable timediscretizations of up to fourth order which are specially tailored for stability when coupled with the pseudospectral method. For this nonlinear problem, we adopt an explicit multi-step Adams-Bashforth approach for the convection term and an implicit Adams-Moulton method for the diffusion term. This approach has the advantage of handling the nonlinear terms in an inexpensive way, while providing the stability associated with implicit methods. However, a naive approach to the time-discretization of the diffusion term (particularly in the third and fourth order cases) yields an unstable method. For this reason, we first determine necessary conditions on the coefficients of the Adams-Moulton method for stability. Using these conditions we then derive methods of up to fourth order which are stable when coupled with the pseudospectral method. For each time-discretization, we prove that when the equation is solved by the pseudospectral method up to some fixed final time T^* , the method is consistent, stable and convergent (to design order) in the H^2 norm. In addition, the maximum norm bound of the numerical solution is automatically obtained, because of the H^2 error estimate and the corresponding Sobolev embedding in 3-D. We thus avoid the use of the inverse inequality in our stability analysis and, as a result, do not require any scaling law between the time step Δt and the space grid size h. Instead, the numerical stability is always preserved provided that Δt and h are bounded by two corresponding given constants over a finite time.

This paper is organized as follows. In Sect. 2 we give a general description of Fourier spectral and pseudospectral differentiation and provide a detailed analysis to bound the collocation interpolation in H^k norms. The first order (in time) semi-implicit scheme is presented and analyzed in Sect. 3. The second, third and fourth order schemes are studied in Sects. 4 and 5, respectively. Finally, some concluding remarks are made in Sect. 6.

2 A Gentle Introduction to Fourier Spectral and Pseudospectral Methods

The Fourier series of a function $f(x, y, z) \in L^2(\Omega)$ with $\Omega = (0, 1)^3$ is defined by

$$f(x, y, z) = \sum_{l,m,n=-\infty}^{\infty} \hat{f}_{l,m,n} e^{2\pi i (lx+my+nz)}$$

with

$$\hat{f}_{l,m,n} = \int_{\Omega} f(x, y, z) \mathrm{e}^{-2\pi \mathrm{i}(lx+my+nz)} dx dy dz.$$

In turn, the truncated series is the projection onto the space \mathcal{B}^N of trigonometric polynomials in x, y, and z of degree up to N, given by

$$\mathcal{P}_N f(x, y, z) = \sum_{l,m,n=-N}^N \hat{f}_{l,m,n} e^{2\pi i (lx+my+nz)}.$$

If f(x, y, z) and all its derivatives up to *m*-th order are continuous and periodic with $|f^{(k)}| \le M$, then the truncated series converges

$$\left\|f(x, y, z) - \mathcal{P}_N f(x, y, z)\right\| \le CMN^{-m},$$

in which $\|\cdot\|$ denotes the L^2 norm.

The L^2 projection operator is one approach to a Fourier series approximation. However, sometimes we want an approximation which matches the function at a given set of points. For this purpose, an interpolation operator \mathcal{I}_N is introduced. Given a uniform 3-D numerical grid with (2N + 1) points in each dimension and a discrete vector function f, where each

point is denoted by (x_i, y_j, z_k) and the corresponding function value is given by $f_{i,j,k}$, the interpolation of the function is

$$(\mathcal{I}_N f)(x, y, z) = \sum_{l,m,n=-N}^{N} \left(\hat{f}_c^N\right)_{l,m,n} e^{2\pi i (lx + my + nz)},$$
(2)

where the $(2N + 1)^3$ pseudospectral coefficients $(\hat{f}_c^N)_{l,m,n}$ are given by the interpolation condition $f_{i,j,k} = (\mathcal{I}_N f)(x_i, y_j, z_k)$. Sometimes we are also interested in the relationship between a continuous function and its interpolation. We want to look at the continuous function that results from evaluating the coefficients by collocation. Given a function f(x, y, z), we compute its collocation coefficients $(\hat{f}_c)_{l,m,n}^N$ based on the 2N + 1 equidistant points in each dimension. In turn, the function $\mathcal{I}_N f(x, y, z)$ is defined to be the continuous expansion based on these coefficients, given by (2). Similary, the interpolation condition $f(x_i, y_j, z_k) = (\mathcal{I}_N f)(x_i, y_j, z_k)$ is satisfied for a continuous function f. See the relevant references [4, 7, 8, 22]. These collocation coefficients can be efficiently computed using the fast Fourier transform (FFT). Note that the pseudospectral coefficients depend on the number of points: increasing N gives a completely different set of coefficients. Also, the pseudospectral coefficients are not equal to the actual Fourier coefficients; the difference between them is known as the aliasing error. In general, $\mathcal{P}_N f(x, y, z) \neq \mathcal{I}_N f(x, y, z)$, and even $\mathcal{P}_N f(x_i, y_i, z_k) \neq \mathcal{I}_N f(x_i, y_i, z_k)$, except of course in the case that $f \in \mathcal{B}^N$.

The Fourier series and the formulas for its projection and interpolation allow us to easily take derivatives in the x, y, or z direction by simply multiplying the appropriate Fourier coefficients $(\hat{f}_c^N)_{l,m,n}$ by $2l\pi i$, $2m\pi i$, or $2n\pi i$, respectively. Furthermore, we can take subsequent derivatives in the same way, so that differentiation in physical space is accomplished via multiplication in Fourier space. As long as f and all is derivatives (up to m-th order) are continuous and periodic on Ω , the convergence of the derivatives of the projection and interpolation is given by

$$\begin{aligned} \left\| \partial^{k} f(x, y, z) - \partial^{k} \mathcal{P}_{N} f(x, y, z) \right\| &\leq \left\| f^{(m)} \right\| N^{k-m}, \quad \text{for } 0 \leq k \leq m, \\ \left\| \partial^{k} f(x, y, z) - \partial^{k} \mathcal{I}_{N} f(x, y, z) \right\| &\leq \left\| f \right\|_{H^{m}} N^{k-m}, \quad \text{for } 0 \leq k \leq m, \ m > \frac{d}{2}. \end{aligned}$$
(3)

Also see the related discussion of approximation theory [6] by Canuto and Quarteroni. Recall that the collocation coefficients $(\hat{f}_c^N)_{l,m,n}$ differ from the actual Fourier coefficients $\hat{f}_{l.m.n}$. Due to this difference, interpolation of the derivative is no longer equal to the derivative of the interpolation.

These properties of the Fourier projection and interpolation form the basis of the Fourier spectral and pseudospectral methods. The Fourier spectral method for (1) relies on the projection operator \mathcal{P}_N : the method is defined by the requirement that the projection of the residual onto the space \mathcal{B}^N will be zero. This requirement produces a system of ordinary differential equations which are then approximated numerically. This approach is known as the Galerkin approach. An alternative to the Galerkin spectral approach is the pseudospectral (or collocation) approach. The Fourier pseudospectral method for (1) relies on the interpolation operator \mathcal{I}_N : the method is defined by the requirement that the interpolation of the residual onto the uniform grid will be zero. Once again, this requirement produces a system of ordinary differential equations which are then integrated numerically.

The major advantage of the collocation method is that it easier to implement, and very efficient due to the fast Fourier transform. The ease of implementation comes from the fact

that the collocation approach is point-wise, which avoids many difficulties when evaluating three dimensional nonlinear terms. On the other hand, the Galerkin spectral method is much easier to analyze, because it does not suffer from aliasing errors. Many works detailing the stability and convergence analysis of spectral methods exist, such as [9, 12, 16, 19, 27, 34, 35, 37, 39, 41, 43, 45, 46]. In this work, we focus on the analysis of the Fourier collocation (or pseudospectral) method applied to (1). Despite the aliasing errors that appear in the collocation method, we are able to establish its stability and convergence properties for a fixed final time.

2.1 Discrete Differentiation

Given a collocation approximation to the function f(x, y, z) at the points x_i, y_j, z_k described above,

$$f(x_i, y_j, z_k) = (\mathcal{I}_N f)_{i,j,k} = \sum_{l,m,n=-N}^{N} (\hat{f}_c^N)_{l,m,n} e^{2\pi i (lx_i + my_j + nz_k)},$$
(4)

we can define the discrete differentiation operators \mathcal{D}_{Nx} , \mathcal{D}_{Ny} , and \mathcal{D}_{Nz} operating on the vector of grid values $\mathbf{f} = f(x_i, y_j, z_k)$. In practice, one may compute the collocation coefficients $(f_c^{\hat{N}})_{l,m,n}$ via FFT, and then multiply them by the correct values (given by $2\pi i l$, $2\pi i m$, $2\pi i n$ in the *x*, *y* and *z* directions, respectively) and perform the inverse FFT. Alternatively, we can view the differentiation operators \mathcal{D}_{Nx} , \mathcal{D}_{Ny} , \mathcal{D}_{Nz} as matrices, and the above process can be seen as a matrix-vector multiplication. Once again, we note that the derivative of the interpolation is not the interpolation of the derivative: $\mathcal{D}_N \mathcal{I}_N f \neq \mathcal{I}_N \mathcal{D}_N f$.

The same process is performed for the second derivatives ∂_x^2 , ∂_y^2 , ∂_z^2 , where this time the collocation coefficients are multiplied by $(-4\pi^2 l^2)$, $(-4\pi^2 m^2)$ and $(-4\pi^2 n^2)$, respectively. Alternatively, the differentiation matrix can be applied twice, i.e. the vector **f** is multiplied by \mathcal{D}_{Nx}^2 for the *x*-derivative, and so on. In turn, we define the discrete Laplacian, gradient and divergence

$$\Delta_{N}\mathbf{f} = \left(\mathcal{D}_{Nx}^{2} + \mathcal{D}_{Ny}^{2} + \mathcal{D}_{Nz}^{2}\right)\mathbf{f},$$

$$\nabla_{N}\mathbf{f} = \begin{pmatrix}\mathcal{D}_{Nx}\mathbf{f}\\\mathcal{D}_{Ny}\mathbf{f}\\\mathcal{D}_{Nz}\mathbf{f}\end{pmatrix}, \qquad \nabla_{N}\cdot\begin{pmatrix}\mathbf{f}\\\mathbf{g}\\\mathbf{h}\end{pmatrix} = \mathcal{D}_{Nx}\mathbf{f} + \mathcal{D}_{Ny}\mathbf{g} + \mathcal{D}_{Nz}\mathbf{h},$$

in the point-wise sense.

2.2 Norms and Inner Products

Since the pseudospectral differentiation is taken at a point-wise level, we need to introduce a discrete L^2 norm and inner product to facilitate the analysis in later sections. Given any periodic grid functions **f** and **g** (over the 3-D numerical grid), we note that these are simply vectors and define the discrete L^2 inner product and norm

$$\|\mathbf{f}\|_{2} = \sqrt{\langle \mathbf{f}, \mathbf{f} \rangle}, \quad \text{with } \langle \mathbf{f}, \mathbf{g} \rangle = \left(\frac{1}{2N+1}\right)^{3} \sum_{i,j,k=0}^{2N} \mathbf{f}_{i,j,k} \mathbf{g}_{i,j,k}.$$
(5)

This discrete L^2 inner product can be computed in Fourier space rather than in physical space, with the help of Parseval's equality:

$$\langle \mathbf{f}, \mathbf{g} \rangle = \sum_{l,m,n=-N}^{N} \left(\hat{f}_{c}^{N} \right)_{l,m,n} \overline{\left(\hat{g}_{c}^{N} \right)_{l,m,n}} = \sum_{l,m,n=-N}^{N} \left(\hat{g}_{c}^{N} \right)_{l,m,n} \overline{\left(\hat{f}_{c}^{N} \right)_{l,m,n}},$$

where $(\hat{f}_c^N)_{l,m,n}$, $(\hat{g}_c^N)_{l,m,n}$ are the Fourier collocation coefficients of the grid functions **f** and **g** in the expansion as in (4).

Furthermore, a detailed calculation shows that the following formulas of integration by parts are also valid at the discrete level:

$$\left\langle \mathbf{f}, \nabla_N \cdot \begin{pmatrix} \mathbf{g}_1 \\ \mathbf{g}_2 \\ \mathbf{g}_3 \end{pmatrix} \right\rangle = -\left\langle \nabla_N \mathbf{f}, \begin{pmatrix} \mathbf{g}_1 \\ \mathbf{g}_2 \\ \mathbf{g}_3 \end{pmatrix} \right\rangle, \qquad \langle \mathbf{f}, \Delta_N \mathbf{g} \rangle = -\langle \nabla_N \mathbf{f}, \nabla_N \mathbf{g} \rangle. \tag{6}$$

2.3 A Preliminary Estimate in Fourier Collocation Space

In this section we state a lemma which will be helpful later in bounding the aliasing error for the nonlinear term. Consider a function $\varphi(x, y, z)$ which is in the space \mathcal{B}^{2N} . Its collocation coefficients $\hat{p}_{l,m,n}^N$ are computed based on the 2N + 1 equidistant points in each dimension. In turn, $\mathcal{I}_N \varphi(x, y, z)$ is given by the continuous expansion based on these coefficients:

$$\mathcal{I}_N\varphi(x, y, z) = \sum_{l,m,n=-N}^N \hat{p}_{l,m,n}^N \mathrm{e}^{2\pi\mathrm{i}(lx+my+nz)}.$$

Note that, because $\varphi(x, y, z) \in \mathcal{B}^{2N}$, the collocation coefficients $\hat{p}_{l,m,n}^N$ are not typically equal to the Fourier coefficients $\hat{\varphi}_{l,m,n}$, so $\mathcal{I}_N \varphi(x, y, z) \neq \mathcal{P}_N \varphi(x, y, z)$.

The following lemma will enable us to obtain an H^m bound of the interpolation of the nonlinear term.

Lemma 1 For any $\varphi \in \mathcal{B}^{2N}$ in dimension *d*, we have

$$\|\mathcal{I}_N\varphi\|_{H^k} \le (\sqrt{2})^d \|\varphi\|_{H^k}.$$
(7)

Proof For simplicity we start from the one dimensional case d = 1. We can write the Fourier expansion of $\varphi \in \mathcal{B}^{2N}$

$$\varphi(x) = \sum_{l=-2N}^{2N} \hat{\varphi}_l \mathrm{e}^{2\pi \mathrm{i} l x},$$

and its interpolation and the corresponding collocation coefficients are given by

$$\mathcal{I}_{N}\varphi(x) = \sum_{l=-N}^{N} \hat{p}_{l}^{N} e^{2\pi i l x}, \quad \text{with } \hat{p}_{l}^{N} = \begin{cases} \hat{\varphi}_{l} + \hat{\varphi}_{l+2N+1}, & \text{if } -N \le l \le -1, \\ \hat{\varphi}_{l}, & \text{if } l = 0, \\ \hat{\varphi}_{l} + \hat{\varphi}_{l-2N-1}, & \text{if } 1 \le l \le N; \end{cases}$$

also see [38] for relevant discussions. Similarly, the Fourier expansions of the *k*-th order derivative of φ and $\mathcal{I}_N \varphi$ are

$$\partial_x^k \varphi(x) = \sum_{l=-2N}^{2N} (2\pi \mathrm{i} l)^k \hat{\varphi}_l \mathrm{e}^{2\pi \mathrm{i} l x}, \qquad \partial_x^k \mathcal{I}_N \varphi(x) = \sum_{l=-N}^N (2\pi \mathrm{i} l)^k \hat{p}_l^N \mathrm{e}^{2\pi \mathrm{i} l x}.$$

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Parseval's equality yields the L^2 and H^k norms of φ and $\mathcal{I}_N \varphi$:

$$\|\varphi\|_{L^2}^2 = \sum_{l=-2N}^{2N} |\hat{\varphi}_l|^2, \qquad \left\|\partial_x^k \varphi\right\|_{L^2}^2 = \sum_{k_1=-2N}^{2N} (2l\pi)^{2k} |\hat{\varphi}_{k_1}|^2, \tag{8}$$

$$\|\mathcal{I}_{N}\varphi\|_{L^{2}}^{2} = \sum_{l=-N}^{N} |\hat{p}_{l}^{N}|^{2}, \qquad \|\partial_{x}^{k}\mathcal{I}_{N}\varphi\|_{L^{2}}^{2} = \sum_{l=-N}^{N} (2l\pi)^{2k} |\hat{p}_{l}^{N}|^{2}.$$
(9)

We can bound the collocation coefficients by

$$\begin{aligned} \left| \hat{p}_{l}^{N} \right|^{2} &= \left| \hat{\varphi}_{l} + \hat{\varphi}_{l+2N} \right|^{2} \leq 2 \left(\left| \hat{\varphi}_{l} \right|^{2} + \left| \hat{\varphi}_{l+2N+1} \right|^{2} \right), & \text{if } -N \leq l \leq -1, \\ \left| \hat{p}_{l}^{N} \right|^{2} &= \left| \hat{\varphi}_{l} + \hat{\varphi}_{l-2N} \right|^{2} \leq 2 \left(\left| \hat{\varphi}_{l} \right|^{2} + \left| \hat{\varphi}_{l-2N-1} \right|^{2} \right), & \text{if } 1 \leq l \leq N, \end{aligned}$$

so that

$$\left\|\mathcal{I}_N\varphi\right\|_{L^2}^2 \leq 2\left\|\varphi\right\|_{L^2}^2,$$

which is exactly Estimate (7) with k = 0.

A more detailed calculation reveals that for $-N \le l \le -1$

$$(2l\pi)^{2k} |\hat{p}_{l}^{N}|^{2} = (2l\pi)^{2k} |\hat{\varphi}_{l} + \hat{\varphi}_{l+2N+1}|^{2}$$

$$\leq 2(2l\pi)^{2k} (|\hat{\varphi}_{l}|^{2} + |\hat{\varphi}_{l+2N+1}|^{2})$$

$$\leq 2 ((2l\pi)^{2k} |\hat{\varphi}_{l}|^{2} + (2(l+2N+1)\pi)^{2k} |\hat{\varphi}_{l+2N+1}|^{2}),$$
since $|l+2N+1| \geq |l|$, for $-N \leq l \leq -1$, (10)

and similarly, for $1 \le l \le N$

$$(2l\pi)^{2k} |\hat{p}_l^N|^2 \le 2((2l\pi)^{2k} |\hat{\varphi}_l|^2 + (2(l-2N)\pi)^{2k} |\hat{\varphi}_{l-2N}|^2),$$

since $|l-2N| \ge |l|$, for $1 \le l \le N$. (11)

Consequently, a combination of (10)–(11) and (8)–(9) results in

$$\sum_{l=-N}^{N} (2l\pi)^{2k} \left| \hat{p}_{l}^{N} \right|^{2} \le 2 \sum_{l=-2N}^{2N} (2l\pi)^{2k} |\hat{\varphi}_{l}|^{2}, \quad \text{i.e. } \left\| \partial_{x}^{k} \mathcal{I}_{N} \varphi \right\|_{L^{2}}^{2} \le 2 \left\| \partial_{x}^{k} \varphi \right\|_{L^{2}}^{2}.$$

Putting this all together

$$\begin{split} \|\mathcal{I}_{N}\varphi\|_{H^{k}}^{2} &= \sum_{q=0}^{k} \left\|\partial_{x}^{q}\mathcal{I}_{N}\varphi\right\|_{L^{2}}^{2} = \sum_{q=0}^{k} \sum_{l=-N}^{N} (2l\pi)^{2q} \left|\hat{p}_{l}^{N}\right|^{2} \\ &\leq \sum_{q=0}^{k} 2\sum_{l=-2N}^{2N} (2l\pi)^{2q} \left|\hat{\varphi}_{l}\right|^{2} = 2\sum_{q=0}^{k} \left\|\partial_{x}^{q}\varphi\right\|_{L^{2}}^{2} = 2\|\varphi\|_{H^{k}}^{2}. \end{split}$$

This completes the proof of (7) for d = 1, for any integer $k \ge 0$. The extension to higher dimensions is straightforward, and the technical details are skipped for brevity of presentation.

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Remark 1 An estimate for the k = 0 case was reported in E's work [44, 45], with the constant given by 3^d . This lemma sharpens the constant to $\sqrt{2}^d$.

Remark 2 We observe that a similar approximation theory result for spectral expansions and interpolations in Sobolev spaces was reported by Canuto and Quarteroni [6],

$$\|\varphi - \mathcal{I}_N \varphi\|_{H^k} \le C N^{k-m} \|\varphi\|_{H^m}, \quad \forall \varphi \in H^m(\Omega),$$

with $0 \le k \le m$ and $m > \frac{d}{2}$; this result is also equivalent to the spectral approximation estimate (3). As a direct consequence, taking k = m results in the same estimate as the above lemma for $k = m > \frac{d}{2} = \frac{3}{2}$ (for 3-D, d = 3). However, due to the additional regularity requirement for interpolation operator analysis, the above estimate does not cover the case of k = 0 or k = 1, which we require for the L^2 and H^1 bound of the nonlinear expansion in our analysis. This H^1 control, corresponding to k = 1 in the above lemma, cannot be covered by the general approximation theory presented by [6], nor, to our knowledge, was it explored in any published work.

3 First Order (in Time) Scheme

The first scheme we consider for Eq. (1), is a first-order in time method which treats the nonlinear convection term explicitly for the sake of numerical convenience, and the diffusion term implicitly to avoid a severe time-step restriction:

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t} + \boldsymbol{u}^n \cdot \nabla_N \boldsymbol{u}^n = \boldsymbol{v} \Delta_N \boldsymbol{u}^{n+1}, \qquad (12)$$

where, for example, the first component of the nonlinear convection is

$$\boldsymbol{u}^n \cdot \nabla_N \boldsymbol{u}^n = \boldsymbol{u}^n \mathcal{D}_{Nx} \boldsymbol{u}^n + \boldsymbol{v}^n \mathcal{D}_{Ny} \boldsymbol{u}^n + \boldsymbol{w}^n \mathcal{D}_{Nz} \boldsymbol{u}^n.$$

Note that the numerical solution \boldsymbol{u} of (12) is a vector function evaluated at discrete grid points. Before the convergence statement of the scheme, we introduce its continuous extension in space, defined by $\boldsymbol{u}_{\Delta t,h}^k = \boldsymbol{u}_N^k$, in which $\boldsymbol{u}_N^k \in \mathcal{B}^N$, $\forall k$, is the continuous version of the discrete grid function \boldsymbol{u}^k , with the interpolation formula given by (4).

Our stability and convergence analysis will bound the error between this spatially continuous version of the numerical solution and the exact solution. To bound this function we will be looking at the $\|\cdot\|_{l^{\infty}(0,T^*;H^2)}$ and $\|\cdot\|_{l^2(0,T^*;H^3)}$ norms. For a semi-discrete function w (continuous in space and discrete in time), we define the first of these norms by

$$\|w\|_{l^{\infty}(0,T^*;H^2)} = \max_{0 \le k \le N_k} \|w^k\|_{H^2}, \quad N_k = \left[\frac{T^*}{\Delta t}\right],$$

i.e., we create a discrete time-dependent function by taking the H^2 norm of the numerical approximation in space for each time step t^k , and then take the maximum of this function over all time steps $0 \le k \le N_k$. For the second norm, we perform a similar operation,

$$\|w\|_{l^2(0,T^*;H^3)} = \sqrt{\Delta t \sum_{k=0}^{N_k} \|w^k\|_{H^3}^2}.$$

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Theorem 1 For any final time $T^* > 0$, assume the exact solution u_e to the 3-D viscous Burgers' equation (1) has a regularity of $H^2(0, T^*; H^{m+3})$ with $m \ge 2$. Denote $u_{\Delta t,h}$ as the continuous (in space) extension of the fully discrete numerical solution given by scheme (12). As $\Delta t, h \to 0$, we have the following convergence result:

$$\|\boldsymbol{u}_{\Delta t,h} - \boldsymbol{u}_e\|_{l^{\infty}(0,T^*;H^2)} + \sqrt{\nu} \|\boldsymbol{u}_{\Delta t,h} - \boldsymbol{u}_e\|_{l^2(0,T^*;H^3)} \le C(\Delta t + h^m),$$
(13)

provided that the time step Δt and the space grid size h are bounded by given constants

$$\Delta t \le L_1(T^*, v), \qquad h \le L_2(T^*, v).$$

Note that the convergence constant in (13) also depend on the exact solution, as well as T^* and v.

The convergence analysis follows a combination of consistency analysis for the collocation scheme (12) and a stability analysis for the numerical error function. In the consistency analysis presented in Sect. 3.1, instead of a direct comparison between the numerical solution and the exact solution, we construct an approximate solution by projecting the exact solution onto \mathcal{B}^N . The consistency analysis shows that such an approximate solution satisfies the numerical scheme up to an $O(\Delta t)$ accuracy in time and a spectral accuracy in space. In the stability and convergence analysis presented in Sect. 3.2, we first make an H^2 a-priori assumption for the numerical error function, which overcomes the difficulty in obtaining an L^{∞} bound for the numerical solution, with an application of 3-D Sobolev embedding. Based on this a-priori assumption, a detailed error estimate can be performed in both L^2 and H^2 norms, with the help of Lemma 1 to bound the aliasing errors associated with the nonlinear terms. Afterward, the H^2 a-priori assumption is recovered at the next time step, due to the error bound in the H^2 norm, so that induction (in time) can be applied.

This approach avoids an application of the inverse inequality. As a result, an unconditional numerical stability (time step vs. spatial grid size) is obtained, and no scaling law is required between Δt and h, as compared with the classical references [1, 5, 11, 19], among others.

3.1 Consistency Analysis

Let

$$\boldsymbol{U}_{N}(\boldsymbol{x},t) = \mathcal{P}_{N}\boldsymbol{u}_{e}(\boldsymbol{x},t). \tag{14}$$

The following approximation estimate is clear from our discussion from Sect. 2:

$$\|\boldsymbol{U}_N - \boldsymbol{u}_e\|_{L^{\infty}(0,T^*;H^r)} \le Ch^m \|\boldsymbol{u}_e\|_{L^{\infty}(0,T^*;H^{m+r})}, \text{ for } r \ge 0.$$

As a result, an application of Sobolev embedding in 3-D gives

$$\|\boldsymbol{U}_N - \boldsymbol{u}_e\|_{L^{\infty}(\Omega)} \le C \|\boldsymbol{U}_N - \boldsymbol{u}_e\|_{H^2} \le Ch^m \|\boldsymbol{u}_e\|_{L^{\infty}(0,T^*;H^{m+2})}, \quad \text{at any fixed time.}$$
(15)

Looking at the time derivative of the projection operator, we observe that

$$\frac{\partial^k}{\partial t^k} \boldsymbol{U}_N(\boldsymbol{x}, t) = \frac{\partial^k}{\partial t^k} \mathcal{P}_N \boldsymbol{u}_e(\boldsymbol{x}, t) = \mathcal{P}_N \frac{\partial^k \boldsymbol{u}_e(\boldsymbol{x}, t)}{\partial t^k};$$
(16)

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in other words, $\partial_t^k U_N$ is the truncation of $\partial_t^k u_e$ for any $k \ge 0$, since projection and differentiation commute. This in turn implies a spectrally accurate approximation of the corresponding temporal derivative:

$$\left\|\partial_t^k (\boldsymbol{U}_N - \boldsymbol{u}_e)\right\|_{L^2} \le Ch^m \left\|\partial_t^k \boldsymbol{u}_e\right\|_{H^m}, \quad \text{for } 0 \le k \le 2.$$
(17)

The bounds on the projection error and its derivatives, namely (15) and (17), indicate that

$$\partial_t \boldsymbol{U}_N + \boldsymbol{U}_N \cdot \nabla \boldsymbol{U}_N - \nu \Delta \boldsymbol{U}_N = \partial_t \boldsymbol{u}_e + \boldsymbol{u}_e \cdot \nabla \boldsymbol{u}_e - \nu \Delta \boldsymbol{u}_e + \boldsymbol{\tau}_1 = \boldsymbol{\tau}_1,$$

with $\|\boldsymbol{\tau}_1\|_{L^2} \le Ch^m$, (18)

in which Hölder's inequality was utilized to estimate the nonlinear term and the last step is based on the fact that u_e is the exact solution. This shows that if the solution u_e satisfies the original viscous Burgers' equation exactly, then its projection U_N will satisfy the PDE up to spectral accuracy.

Now consider the time discrete version of the equation. The temporal grid is discretized using equidistant points $t^n = n\Delta t$. We denote $U_N^n(\mathbf{x}) = \mathcal{P}_N \mathbf{u}_e(\mathbf{x}, t^n)$. Recall the $U_N^n \in \mathcal{B}^N$, so that it is equal to its interpolation, and its derivatives can be computed exactly by the collocation differentiation operators ∇_N and Δ_N .

Moreover, for the approximate solution U_N^n , we define its vector grid function U^n as its interpolation: $U_{i,i,k}^n = U_N^n(x_i, y_j, z_k)$. A detailed error estimate indicates that

$$\boldsymbol{U}^{n} \cdot \nabla_{N} \boldsymbol{U}^{n} = \boldsymbol{U}_{N}^{n} \cdot \nabla \boldsymbol{U}_{N}^{n}, \qquad \Delta_{N} \boldsymbol{U}^{n+1} = \Delta \boldsymbol{U}_{N}^{n+1}, \quad \text{at } (i, j, k), \text{ since } \boldsymbol{U}_{N}^{n} = \mathcal{I}_{N} \boldsymbol{U}^{n},$$
(19)

$$\Delta \boldsymbol{U}_{N}^{n+1} = \Delta \boldsymbol{U}_{N}^{n} + \boldsymbol{\tau}_{2}^{n}, \quad \text{with } \|\boldsymbol{\tau}_{2}\|_{l^{2}(0,T^{*};L^{2})} \leq C \Delta t \|\boldsymbol{U}_{N}\|_{H^{1}(0,T^{*};H^{2})} \leq C \Delta t, \qquad (20)$$

where L_h^2 denotes the discrete L^2 norm given by (5). For the temporal discretization term, we start from the following estimate

$$\frac{U_N^{n+1} - U_N^n}{\Delta t} = \partial_t U_N(\cdot, t^n) + \tau_3^n(\cdot), \quad \text{with } \|\tau_3(\cdot)\|_{l^2(0,T^*)} \le C \Delta t \|U_N(\cdot)\|_{H^2(0,T^*)},$$
(21)

at a point-wise level (in space), in which the derivation is based on an integral form of Taylor's formula. Furthermore, by the observation (16), we arrive at

$$\|\boldsymbol{\tau}_{3}\|_{l^{2}(0,T^{*};L^{2}(\Omega))} \leq C\Delta t \|\partial_{l}^{2}\boldsymbol{U}_{N}\|_{L^{2}(0,T^{*};L^{2}(\Omega))} \leq C\Delta t \|\partial_{l}^{2}\boldsymbol{u}_{e}\|_{L^{2}(0,T^{*};L^{2}(\Omega))} \leq C\Delta t.$$
(22)

Consequently, a combination of (18) and (19), (20), (21), (22) implies the consistency of the approximate solution U:

$$\frac{\boldsymbol{U}^{n+1} - \boldsymbol{U}^n}{\Delta t} + \boldsymbol{U}^n \cdot \nabla_N \boldsymbol{U}^n - \nu \Delta_N \boldsymbol{U}^{n+1} = \boldsymbol{\tau}^n,$$

with $\boldsymbol{\tau} = I_N(\boldsymbol{\tau}_1 + \boldsymbol{\tau}_2 + \boldsymbol{\tau}_3), \quad \|\boldsymbol{\tau}\|_{l^2(0,T^*;L^2_h)} \le C(\Delta t + h^m),$ (23)

with I_N the standard operator to project a continuous function onto the discrete grid point. In other words, the projection of the exact solution satisfies the numerical scheme (12) up to an $O(\Delta t + h^m)$ truncation error. In addition, we also observe that the H^1 norm of τ is also bounded at the consistency order, namely

$$\|\boldsymbol{\tau}\|_{l^{2}(0,T^{*};H_{h}^{1})} := \sqrt{\Delta t \sum_{k=0}^{N_{k}} \|\boldsymbol{\tau}_{N}^{k}\|_{H^{1}}^{2}} \leq C(\Delta t + h^{m}),$$
(24)

where $\tau_N^k \in \mathcal{B}^N$ is the continuous version of τ^k . Such an estimate is derived based on higher order asymptotic expansions. In fact, this discrete H^1 truncation error bound is needed in the $l^{\infty}(0, T^*; H^2)$ error estimate as presented in later sections; such a bound is derived based on H^1 analysis of τ_1, τ_2 and τ_3 . The details are skipped for simplicity of presentation.

3.2 Stability and Convergence Analysis

The point-wise numerical error grid function is given by

$$\boldsymbol{e}_{i,j,k}^{n} = \boldsymbol{U}_{i,j,k}^{n} - \boldsymbol{u}_{i,j,k}^{n}.$$
(25)

The difference between scheme (12) and the consistency (23) gives

$$\frac{\boldsymbol{e}^{n+1}-\boldsymbol{e}^n}{\Delta t}+\boldsymbol{e}^n\cdot\nabla_N\boldsymbol{U}^n+\boldsymbol{u}^n\cdot\nabla_N\boldsymbol{e}^n=\boldsymbol{\nu}\Delta_N\boldsymbol{e}^{n+1}+\boldsymbol{\tau}^n. \tag{26}$$

To facilitate the presentation below, we denote $u_N^n \in \mathcal{B}^N$ and $e_N^n \in \mathcal{B}^N$, as the continuous version of the numerical solution u^n and e^n , respectively, with the interpolation formula given by (4).

The constructed approximate solution has a $W^{2,\infty}$ bound

$$\|U_N\|_{L^{\infty}(0,T^*;W^{2,\infty})} \le C^*, \quad \text{i.e.} \ \|U_N^n\|_{L^{\infty}} \le C^*, \ \|\nabla U_N^n\|_{L^{\infty}} \le C^*, \ \|\nabla (\nabla U_N^n)\|_{L^{\infty}} \le C^*,$$
(27)

for any $n \ge 0$, which comes from the regularity of the constructed solution.

3.2.1 An A-priori H² Assumption

We assume a-priori that the numerical error function has an H^2 bound at time step t^n :

$$\left\|\boldsymbol{e}_{N}^{n}\right\|_{H^{2}} \leq 1, \quad \text{with } \boldsymbol{e}_{N}^{n} = \mathcal{I}_{N}\boldsymbol{e}^{n}, \tag{28}$$

so that the L^{∞} bound for the numerical solution at t^n can be obtained as

$$\|\boldsymbol{u}_{N}^{n}\|_{H^{2}} = \|\boldsymbol{U}_{N}^{n} - \boldsymbol{e}_{N}^{n}\|_{H^{2}} \le \|\boldsymbol{U}_{N}^{n}\|_{H^{2}} + \|\boldsymbol{e}_{N}^{n}\|_{H^{2}} \le C^{*} + 1 := \tilde{C}_{0},$$

$$\|\boldsymbol{u}^{n}\|_{\infty} \le \|\boldsymbol{u}_{N}^{n}\|_{L^{\infty}} \le C \|\boldsymbol{u}_{N}^{n}\|_{H^{2}} \le C\tilde{C}_{0} := \tilde{C}_{1}.$$
(29)

3.2.2 Leading Order Error Estimate: In $l^{\infty}(0, T^*; L^2) \cap l^2(0, T^*; H^1)$ Norm

Lemma 2 Under the a-priori assumption (28), the numerical error function for the first order scheme (12) satisfies

$$\|\boldsymbol{e}^{n+1}\|_{2} + \sqrt{\nu \Delta t} \sum_{k=1}^{n+1} \|\nabla_{N} \boldsymbol{e}^{k}\|_{2}^{2} \leq M_{1} (\Delta t + h^{m}).$$
(30)

Proof Taking a discrete L^2 inner product of (26) with $2e^{n+1}$ yields

$$\langle \boldsymbol{e}^{n+1} - \boldsymbol{e}^n, 2\boldsymbol{e}^{n+1} \rangle - 2\nu \Delta t \langle \Delta_N \boldsymbol{e}^{n+1}, \boldsymbol{e}^{n+1} \rangle = -2\Delta t \langle \boldsymbol{e}^n \cdot \nabla_N \boldsymbol{U}^n, \boldsymbol{e}^{n+1} \rangle - 2\Delta t \langle \boldsymbol{u}^n \cdot \nabla_N \boldsymbol{e}^n, \boldsymbol{e}^{n+1} \rangle + 2\Delta t \langle \boldsymbol{\tau}^n, \boldsymbol{e}^{n+1} \rangle.$$
(31)

The time marching term and the truncation error term can be handled in a straightforward way:

$$\langle \boldsymbol{e}^{n+1} - \boldsymbol{e}^n, 2\boldsymbol{e}^{n+1} \rangle = \| \boldsymbol{e}^{n+1} \|_2^2 - \| \boldsymbol{e}^n \|_2^2 + \| \boldsymbol{e}^{n+1} - \boldsymbol{e}^n \|_2^2,$$
 (32)

$$2\langle \boldsymbol{\tau}^{n}, \boldsymbol{e}^{n+1} \rangle \leq \| \boldsymbol{\tau}^{n} \|_{2}^{2} + \| \boldsymbol{e}^{n+1} \|_{2}^{2},$$
(33)

in which a discrete Cauchy inequality was utilized. A discrete version of the integration by parts formula (6) can be applied to analyze the diffusion term:

$$-2\langle \Delta_N \boldsymbol{e}^{n+1}, \boldsymbol{e}^{n+1} \rangle = 2\langle \nabla_N \boldsymbol{e}^{n+1}, \nabla_N \boldsymbol{e}^{n+1} \rangle = 2 \| \nabla_N \boldsymbol{e}^{n+1} \|_2^2.$$
(34)

For the numerical error of the nonlinear convection, we see that the first term can be handled by the Cauchy inequality, with the $W^{1,\infty}$ bound of the approximate solution given by (27):

$$-2\langle \boldsymbol{e}^{n} \cdot \nabla_{N} \boldsymbol{U}^{n}, \boldsymbol{e}^{n+1} \rangle \leq 2 \| \nabla_{N} \boldsymbol{U}^{n} \|_{\infty} \cdot \| \boldsymbol{e}^{n} \|_{2} \cdot \| \boldsymbol{e}^{n+1} \|_{2}$$
$$\leq 2C^{*} \| \boldsymbol{e}^{n} \|_{2} \cdot \| \boldsymbol{e}^{n+1} \|_{2} \leq C^{*} \| \boldsymbol{e}^{n} \|_{2}^{2} + C^{*} \| \boldsymbol{e}^{n+1} \|_{2}^{2}.$$
(35)

Similar analysis can be applied to the second nonlinear error term:

$$-2\langle \boldsymbol{u}^{n} \cdot \nabla_{N} \boldsymbol{e}^{n}, \boldsymbol{e}^{n+1} \rangle \leq 2 \| \boldsymbol{u}^{n} \|_{\infty} \cdot \| \nabla_{N} \boldsymbol{e}^{n} \|_{2} \cdot \| \boldsymbol{e}^{n+1} \|_{2}$$

$$\leq 2 \tilde{C}_{1} \| \nabla_{N} \boldsymbol{e}^{n} \|_{2} \cdot \| \boldsymbol{e}^{n+1} \|_{2} \leq \nu \| \nabla_{N} \boldsymbol{e}^{n} \|_{2}^{2} + \frac{\tilde{C}_{1}^{2}}{\nu} \| \boldsymbol{e}^{n+1} \|_{2}^{2}, \quad (36)$$

in which the L^{∞} a-priori bound (29) was used in the second step.

As a result, a substitution of (32), (33), (34), (35) and (36) into (31) gives

$$\|\boldsymbol{e}^{n+1}\|_{2}^{2} - \|\boldsymbol{e}^{n}\|_{2}^{2} + \|\boldsymbol{e}^{n+1} - \boldsymbol{e}^{n}\|_{2}^{2} + 2\nu\Delta t \|\nabla_{N}\boldsymbol{e}^{n+1}\|_{2}^{2}$$

$$\leq \nu\Delta t \|\nabla_{N}\boldsymbol{e}^{n}\|_{2}^{2} + \left(\frac{\tilde{C}_{1}^{2}}{\nu} + C^{*} + 1\right)\Delta t \|\boldsymbol{e}^{n+1}\|_{2}^{2} + C^{*}\Delta t \|\boldsymbol{e}^{n}\|_{2}^{2} + \Delta t \|\boldsymbol{\tau}^{n}\|_{2}^{2}.$$

Summing in time gives

$$\begin{aligned} \|\boldsymbol{e}^{n+1}\|_{2}^{2} + \sum_{k=0}^{n} \|\boldsymbol{e}^{k+1} - \boldsymbol{e}^{k}\|_{2}^{2} + \nu \Delta t \sum_{k=1}^{n+1} \|\nabla_{N}\boldsymbol{e}^{k}\|_{2}^{2} \\ &\leq \tilde{C}_{2}\Delta t \sum_{k=0}^{n+1} \|\boldsymbol{e}^{k}\|_{2}^{2} + \Delta t \sum_{k=0}^{n} \|\boldsymbol{\tau}^{n}\|_{2}^{2} + \nu \Delta t \|\nabla_{N}\boldsymbol{e}^{0}\|_{2}^{2} + Ch^{2m} \\ &\leq \tilde{C}_{2}\Delta t \sum_{k=0}^{n+1} \|\boldsymbol{e}^{k}\|_{2}^{2} + \Delta t \sum_{k=0}^{n} \|\boldsymbol{\tau}^{n}\|_{2}^{2} + Ch^{2m}, \end{aligned}$$

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with $\tilde{C}_2 = \frac{\tilde{C}_1^2}{\nu} + 2C^* + 1$. Note that we used the fact $\|e^0\|_{H_h^1} \leq Ch^m$, due to the collocation spectral approximation of the initial data. An application of the discrete Gronwall inequality leads to (30), with $M_1 = Ce^{\frac{1}{2}\tilde{C}_2T^*}$. Also note that the truncation error estimate (23) was used. This in turn gives the $l^{\infty}(0, T^*; L^2) \cap l^2(0, T^*; H^1)$ error estimate for the numerical scheme, under the a-priori $H^{\frac{3}{2}+\delta}$ assumption (28).

It is observed that the L^2 convergence (30) is based on the a-priori H^2 assumption (28) for the numerical solution. We need an H^2 error estimate to recover this assumption.

3.2.3 Higher Order Error Estimate: In $l^{\infty}(0, T^*; H^2) \cap l^2(0, T^*; H^3)$ Norm

Taking a discrete L^2 inner product of (26) with $2\Delta_N^2 e^{n+1}$ yields

$$2\langle \boldsymbol{e}^{n+1} - \boldsymbol{e}^{n}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle - 2\nu \Delta t \langle \Delta_{N} \boldsymbol{e}^{n+1}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle$$

= $2\Delta t \left(-\langle \boldsymbol{e}^{n} \cdot \nabla_{N} \boldsymbol{U}^{n}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle - \langle \boldsymbol{u}^{n} \cdot \nabla_{N} \boldsymbol{e}^{n}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle + \langle \boldsymbol{\tau}^{n}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle \right).$ (37)

The time marching term, truncation error term and the diffusion term can be analyzed as

$$2\langle \boldsymbol{e}^{n+1} - \boldsymbol{e}^n, \Delta_N^2 \boldsymbol{e}^{n+1} \rangle = \|\Delta_N \boldsymbol{e}^{n+1}\|_2^2 - \|\Delta_N \boldsymbol{e}^n\|_2^2 + \|\Delta_N (\boldsymbol{e}^{n+1} - \boldsymbol{e}^n)\|_2^2,$$
(38)

$$2\langle \boldsymbol{\tau}^{n}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle = -2\langle \nabla_{N} \boldsymbol{\tau}^{n}, \nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1} \rangle \leq \frac{4}{\nu} \| \nabla_{N} \boldsymbol{\tau}^{n} \|_{2}^{2} + \frac{1}{4} \nu \| \nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1} \|_{2}^{2},$$
(39)

$$-2\langle \Delta_N \boldsymbol{e}^{n+1}, \Delta_N^2 \boldsymbol{e}^{n+1} \rangle = 2\langle \nabla_N \Delta_N \boldsymbol{e}^{n+1}, \nabla_N \Delta_N \boldsymbol{e}^{n+1} \rangle = 2 \| \nabla_N \Delta_N \boldsymbol{e}^{n+1} \|_2^2.$$
(40)

Lemma 3 Under the a-priori assumption (28), we have the following estimates for the nonlinear error terms

$$-2\langle \boldsymbol{e}^{n} \cdot \nabla_{N} \boldsymbol{U}^{n}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle \leq \frac{1}{2} \nu \| \nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1} \|_{2}^{2} + \frac{96(C^{*})^{2}}{\nu} (\| \nabla_{N} \boldsymbol{e}^{n} \|_{2}^{2} + \| \boldsymbol{e}^{n} \|_{2}^{2}), \quad (41)$$

$$-2\langle \boldsymbol{u}^{n} \cdot \nabla_{N} \boldsymbol{e}^{n}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle \leq \frac{1}{2} \nu \left\| \nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1} \right\|_{2}^{2} + \frac{C \tilde{C}_{1}^{2}}{\nu} \left\| \Delta_{N} \boldsymbol{e}^{n} \right\|_{2}^{2}.$$

$$\tag{42}$$

Proof We start with an application of summation by parts to the first term:

$$-2\langle \boldsymbol{e}^{n}\cdot\nabla_{N}\boldsymbol{U}^{n},\Delta_{N}^{2}\boldsymbol{e}^{n+1}\rangle = 2\langle\nabla_{N}(\boldsymbol{e}^{n}\cdot\nabla_{N}\boldsymbol{U}^{n}),\nabla_{N}\Delta_{N}\boldsymbol{e}^{n+1}\rangle.$$
(43)

The remaining work is focused on the nonlinear expansion of $\nabla_N(e^n \cdot \nabla_N U^n)$. For simplicity of presentation, we only look at the first row $\nabla_N(e^n \cdot \nabla_N U^n)$; the two other rows, $\nabla_N(e^n \cdot \nabla_N V^n)$ and $\nabla_N(e^n \cdot \nabla_N W^n)$, can be handled in the same way. Recall that $e_N^n \in \mathcal{B}^N$ is the continuous version of the discrete grid error function e^n , as in (4). It is obvious that

$$\left\|\nabla_{N}\left(\boldsymbol{e}^{n}\cdot\nabla_{N}U^{n}\right)\right\|_{2}=\left\|\nabla\left(\mathcal{I}_{N}\left(\boldsymbol{e}_{N}^{n}\cdot\nabla U_{N}^{n}\right)\right)\right\|_{L^{2}}\leq2\sqrt{2}\left\|\nabla\left(\boldsymbol{e}_{N}^{n}\cdot\nabla U_{N}^{n}\right)\right\|_{L^{2}}.$$
(44)

The first step is based on the fact that e^n , $\nabla_N U^n$ and e^n_N , ∇U^n_N have the same interpolation values. Lemma 1 was applied in the second step, due to the fact that $e^n_N \cdot \nabla U^n_N \in \mathcal{B}^{2N}$. The advantage of this inequality is that the right hand side norm is measured in continuous space. Subsequently, a detailed Sobolev space expansion and applications of Hölder's inequality show that

$$\left\|\nabla\left(\boldsymbol{e}_{N}^{n}\cdot\nabla U_{N}^{n}\right)\right\|_{L^{2}}=\left\|\nabla U_{N}^{n}\cdot\nabla\boldsymbol{e}_{N}^{n}+\boldsymbol{e}_{N}^{n}\cdot\nabla\left(\nabla U_{N}^{n}\right)\right\|_{L^{2}}$$

$$\leq \left\| \nabla U_{N}^{n} \cdot \nabla \boldsymbol{e}_{N}^{n} \right\|_{L^{2}} + \left\| \boldsymbol{e}_{N}^{n} \cdot \nabla (\nabla U_{N}^{n}) \right\|_{L^{2}}$$

$$\leq \left\| \nabla U_{N}^{n} \right\|_{L^{\infty}} \cdot \left\| \nabla \boldsymbol{e}_{N}^{n} \right\|_{L^{2}} + \left\| \boldsymbol{e}_{N}^{n} \right\|_{L^{2}} \cdot \left\| \nabla (\nabla U_{N}^{n}) \right\|_{L^{\infty}}$$

$$\leq C^{*} \left(\left\| \nabla \boldsymbol{e}_{N}^{n} \right\|_{L^{2}} + \left\| \boldsymbol{e}_{N}^{n} \right\|_{L^{2}} \right) = C^{*} \left(\left\| \nabla_{N} \boldsymbol{e}^{n} \right\|_{2} + \left\| \boldsymbol{e}^{n} \right\|_{2} \right),$$

with the regularity fact (27) applied in the last step. Its combination with (44) yields

$$\left\|\nabla_{N}\left(\boldsymbol{e}^{n}\cdot\nabla_{N}U^{n}\right)\right\|_{2}\leq 2\sqrt{2}C^{*}\left(\left\|\nabla_{N}\boldsymbol{e}^{n}\right\|_{2}+\left\|\boldsymbol{e}^{n}\right\|_{2}\right),$$

which in turn also gives

$$\left\|\nabla_{N}\left(\boldsymbol{e}^{n}\cdot\nabla_{N}\boldsymbol{U}^{n}\right)\right\|_{2}\leq 2\sqrt{6}C^{*}\left(\left\|\nabla_{N}\boldsymbol{e}^{n}\right\|_{2}+\left\|\boldsymbol{e}^{n}\right\|_{2}\right).$$

Going back to (43), we get (41), the estimate for the first nonlinear convection error term:

$$-2\langle \boldsymbol{e}^{n} \cdot \nabla_{N} \boldsymbol{U}^{n}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle \leq 4\sqrt{6}C^{*}(\|\nabla_{N} \boldsymbol{e}^{n}\|_{2} + \|\boldsymbol{e}^{n}\|_{2}) \cdot \|\nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1}\|_{2}$$
$$\leq \frac{1}{2}\nu \|\nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1}\|_{2}^{2} + \frac{48(C^{*})^{2}}{\nu}(\|\nabla_{N} \boldsymbol{e}^{n}\|_{2}^{2} + \|\boldsymbol{e}^{n}\|_{2}^{2}).$$

The analysis of the other nonlinear convection error term also starts from the summation by parts:

$$-2\langle \boldsymbol{u}^{n}\cdot\nabla_{N}\boldsymbol{e}^{n},\Delta_{N}^{2}\boldsymbol{e}^{n+1}\rangle = 2\langle\nabla_{N}(\boldsymbol{u}^{n}\cdot\nabla_{N}\boldsymbol{e}^{n}),\nabla_{N}\Delta_{N}\boldsymbol{e}^{n+1}\rangle.$$
(45)

Similarly, Lemma 1 has to be utilized to deal with the nonlinear expansion of $\nabla_N(\boldsymbol{u}^n \cdot \nabla_N \boldsymbol{e}^n)$ in collocation Fourier space. The detailed estimates are given below.

$$\begin{split} \left\| \nabla_{N} \left(\boldsymbol{u}^{n} \cdot \nabla_{N} \boldsymbol{e}^{n} \right) \right\|_{2} &= \left\| \nabla \left(\mathcal{I}_{N} \left(\boldsymbol{u}_{N}^{n} \cdot \nabla \boldsymbol{e}_{N}^{n} \right) \right) \right\|_{L^{2}} \leq 2\sqrt{2} \left\| \nabla \left(\boldsymbol{u}_{N}^{n} \cdot \nabla \boldsymbol{e}_{N}^{n} \right) \right\|_{L^{2}}, \\ \left\| \nabla \left(\boldsymbol{u}_{N}^{n} \cdot \nabla \boldsymbol{e}_{N}^{n} \right) \right\|_{L^{2}} &= \left\| \nabla \boldsymbol{e}_{N}^{n} \otimes \nabla \boldsymbol{u}_{N}^{n} + \boldsymbol{u}_{N}^{n} \cdot \nabla \left(\nabla \boldsymbol{e}_{N}^{n} \right) \right\|_{L^{2}} \\ &\leq \left\| \nabla \boldsymbol{e}_{N}^{n} \otimes \nabla \boldsymbol{u}_{N}^{n} \right\|_{L^{2}} + \left\| \boldsymbol{u}_{N}^{n} \cdot \nabla \left(\nabla \boldsymbol{e}_{N}^{n} \right) \right\|_{L^{2}} \\ &\leq \left\| \nabla \boldsymbol{u}_{N}^{n} \right\|_{L^{3}} \cdot \left\| \nabla \boldsymbol{e}_{N}^{n} \right\|_{L^{6}} + \left\| \boldsymbol{u}_{N}^{n} \right\|_{L^{\infty}} \cdot \left\| \nabla \left(\nabla \boldsymbol{e}_{N}^{n} \right) \right\|_{L^{2}} \\ &\leq C \tilde{C}_{1} \left\| \Delta \boldsymbol{e}_{N}^{n} \right\|_{L^{2}} = C \tilde{C}_{1} \left\| \Delta \mathbf{n} \boldsymbol{e}^{n} \right\|_{2}. \end{split}$$

Note that the a-priori assumption (28)–(29), combined with the following 3-D Sobolev embedding and elliptic regularity were used in the last step:

$$\begin{aligned} \|\nabla \boldsymbol{u}_{N}^{n}\|_{L^{3}} &\leq C \|\boldsymbol{u}_{N}^{n}\|_{H^{\frac{3}{2}}} \leq C\tilde{C}_{1}, \quad \|\nabla \boldsymbol{e}_{N}^{n}\|_{L^{6}} \leq C \|\Delta \boldsymbol{e}_{N}^{n}\|_{L^{2}}, \\ \|\boldsymbol{u}_{N}^{n}\|_{L^{\infty}} &\leq \tilde{C}_{1}, \quad \|\nabla (\nabla \boldsymbol{e}_{N}^{n})\|_{L^{2}} \leq C \|\Delta \boldsymbol{e}_{N}^{n}\|_{L^{2}}. \end{aligned}$$

This in turn shows that

$$\left\|\nabla_{N}\left(\boldsymbol{u}^{n}\cdot\nabla_{N}\boldsymbol{e}^{n}\right)\right\|_{2}\leq 2\sqrt{2}\left\|\nabla\left(\boldsymbol{u}_{N}^{n}\cdot\nabla\boldsymbol{e}_{N}^{n}\right)\right\|_{L^{2}}\leq C\tilde{C}_{1}\left\|\Delta_{N}\boldsymbol{e}^{n}\right\|_{2}.$$

Going back to (45), we arrive at (42), the second part of Lemma 3:

$$-2\langle \boldsymbol{u}^{n} \cdot \nabla_{N} \boldsymbol{e}^{n}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle \leq C \tilde{C}_{1} \| \Delta_{N} \boldsymbol{e}^{n} \|_{2} \cdot \| \nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1} \|_{2}$$
$$\leq \frac{1}{2} \nu \| \nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1} \|_{2}^{2} + \frac{C \tilde{C}_{1}^{2}}{\nu} \| \Delta_{N} \boldsymbol{e}^{n} \|_{2}^{2}. \qquad \Box$$

A substitution of (38)-(40) and Lemma 3 into (37) indicates that

$$\begin{split} \left\| \Delta_{N} \boldsymbol{e}^{n+1} \right\|_{2}^{2} &= \left\| \Delta_{N} \boldsymbol{e}^{n} \right\|_{2}^{2} + \left\| \Delta_{N} \left(\boldsymbol{e}^{n+1} - \boldsymbol{e}^{n} \right) \right\|_{2}^{2} + \frac{3}{4} \nu \Delta t \left\| \nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1} \right\|_{2}^{2} \\ &\leq \frac{C \tilde{C}_{1}^{2} \Delta t}{\nu} \left\| \Delta_{N} \boldsymbol{e}^{n} \right\|_{2}^{2} + \frac{48 (C^{*})^{2} \Delta t}{\nu} \left(\left\| \nabla_{N} \boldsymbol{e}^{n} \right\|_{2}^{2} + \left\| \boldsymbol{e}^{n} \right\|_{2}^{2} \right) + \frac{4 \Delta t}{\nu} \left\| \nabla_{N} \boldsymbol{\tau}^{n} \right\|_{2}^{2}, \\ &\leq \frac{C (\tilde{C}_{1}^{2} + (C^{*})^{2}) \Delta t}{\nu} \left\| \Delta_{N} \boldsymbol{e}^{n} \right\|_{2}^{2} + \frac{(48 (C^{*})^{2} \tilde{C}_{3} + C M_{1}) \Delta t}{\nu} \left(\Delta t + h^{m} \right)^{2} + \frac{4 \Delta t}{\nu} \left\| \nabla_{N} \boldsymbol{\tau}^{n} \right\|_{2}^{2}. \end{split}$$

in which the leading L^2 convergence (30) for the numerical scheme, combined with the elliptic regularity: $\|\nabla_N e^n\|_2 \le C_3 \|\Delta_N e^n\|_2$, was used in the derivation. In turn, applying the discrete Gronwall inequality and using the H^1 consistency (24) lead to

$$\begin{split} \left\| \Delta_{N} \boldsymbol{e}^{n+1} \right\|_{2}^{2} + \sum_{k=0}^{n} \left\| \Delta_{N} \left(\boldsymbol{e}^{k+1} - \boldsymbol{e}^{k} \right) \right\|_{2}^{2} + \frac{3}{4} \nu \Delta t \sum_{k=1}^{n+1} \left\| \nabla_{N} \Delta_{N} \boldsymbol{e}^{k} \right\|_{2}^{2} \\ & \leq \frac{C(48(C^{*})^{2} \tilde{C}_{3} + CM_{1})}{\nu} \boldsymbol{e}^{\tilde{C}_{5}T^{*}} \left(\Delta t + h^{m} \right)^{2} \leq M_{2}^{2} \left(\Delta t + h^{m} \right)^{2}, \end{split}$$

with $\tilde{C}_5 = \frac{C(\tilde{C}_1^2 + (C^*)^2)}{\nu}$, $M_2^2 = \frac{C(48(C^*)^2 \tilde{C}_3 + CM_1)}{\nu} e^{\tilde{C}_5 T^*}$. Therefore, the H^2 error estimate for the numerical scheme is obtained from the following elliptic regularity:

$$\|\boldsymbol{e}_{N}^{n+1}\|_{H^{2}} \leq C(\|\boldsymbol{e}_{N}^{n+1}\|_{L^{2}} + \|\Delta \boldsymbol{e}_{N}^{n+1}\|_{L^{2}})$$

$$\leq \tilde{C}_{6}(\Delta t + h^{m}), \quad \tilde{C}_{6} = C(M_{1} + M_{2}).$$
(46)

As a direct consequence, the point-wise convergence of the numerical scheme is established by an application of 3-D Sobolev embedding:

$$\|\boldsymbol{e}^{n+1}\|_{\infty} \leq \|\boldsymbol{e}^{n+1}_N\|_{L^{\infty}} \leq C \|\boldsymbol{e}^{n+1}_N\|_{H^2} \leq C (M_1 + M_2) (\Delta t + h^m).$$

3.2.4 Recovery of the H^2 A-priori Bound (28)

With the help of the H^2 error estimate (46), we see that the a-priori H^2 bound (28) is also valid for the numerical error vector e^{n+1} at time step t^{n+1} provided that

$$\Delta t \leq (\tilde{C}_6)^{-1}, \qquad h \leq (\tilde{C}_6)^{-\frac{1}{m}}, \quad \text{with } \tilde{C}_6 \text{ dependent on } \nu \text{ and } \exp(T^*).$$

This completes the $L^{\infty}(0, T^*; H^2)$ convergence analysis, and the proof of Theorem 1.

Remark 3 In addition to the standard L^2 convergence analysis based on the L^{∞} a-priori assumption for the numerical solution, an H^2 error estimate is performed in this work. Such an approach avoids an application of the inverse inequality for a discrete function $f: ||f||_{\infty} \le ch^{-d/2} ||f||_2$ (*d* is the dimension), which usually leads to a time step constraint $\Delta t \le Ch^{d/2}$.

It is also noticed that, with an application of the inverse inequality, such a constraint could be relaxed with either a higher order numerical accuracy in time or a higher order asymptotic consistency analysis. This approach usually results in a more relaxed constraint: $\Delta t^k \leq Ch^{d/2}$, in which k is the order of accuracy in time. See the related discussions in [5, 19], etc. However, a constraint between Δt and h would not vanish, unless an error estimate in a Sobolev norm stronger than $H^{\frac{d}{2}}$ is obtained, as presented in this work.

Remark 4 In fact, the H^2 a-priori assumption (28) for the numerical error can be replaced by an $H^{\frac{3}{2}+\delta}$ assumption for any $\delta > 0$, due to the Sobolev embedding in 3-D.

4 Second Order (in Time) Scheme

To derive a second order scheme, we use a similar semi-implicit approach. As before, the nonlinear term is updated explicitly. For the convection term we use a standard second order Adams-Bashforth extrapolation formula, which involves the numerical solutions at time node points t^n , t^{n-1} , with well-known coefficients 3/2 and -1/2, respectively. The diffusion term is treated implicitly, using a second order Adams-Moulton interpolation. However, we do not use the standard second order formula, as this leads to difficulties in the stability analysis. Instead, we look for an Adams-Moulton interpolation such that the diffusion term is more focused on the time step t^{n+1} , i.e., the coefficient at time step t^{n+1} dominates the sum of all other diffusion coefficients. We discovered that the Adams-Moulton interpolation which involves the time node points t^{n+1} and t^{n-1} gives the corresponding coefficients as 3/4, 1/4, respectively, which satisfies the unconditional stability condition. Therefore, we formulate the fully discrete scheme:

$$\frac{u^{n+1} - u^n}{\Delta t} + \frac{3}{2}u^n \cdot \nabla_N u^n - \frac{1}{2}u^{n-1} \cdot \nabla_N u^{n-1} = \nu \Delta_N \left(\frac{3}{4}u^{n+1} + \frac{1}{4}u^{n-1}\right).$$
(47)

Our main result, proven in the subsequent subsections, is as follows.

Theorem 2 For any final time $T^* > 0$, assume the exact solution u_e to the 3-D viscous Burgers' equation (1) has a regularity of $H^3(0, T^*; H^{m+3})$ with $m \ge 2$. Denote $u_{\Delta t,h}$ as the continuous (in space) extension of the fully discrete numerical solution given by scheme (47). As $\Delta t, h \to 0$, we have the following convergence result:

$$\|\boldsymbol{u}_{\Delta t,h} - \boldsymbol{u}_e\|_{l^{\infty}(0,T^*;H^2)} + \sqrt{\nu} \|\boldsymbol{u}_{\Delta t,h} - \boldsymbol{u}_e\|_{l^2(0,T^*;H^3)} \le C(\Delta t^2 + h^m),$$
(48)

provided that the time step Δt and grid size h are bounded by given constants

$$\Delta t \leq L_3(T^*, \nu), \qquad h \leq L_4(T^*, \nu).$$

Note that the convergence constants in (48) also depend on the exact solution, as well as T^* and v.

4.1 Consistency Analysis

Again, denote the approximate solution $U_N(\mathbf{x}, t)$ as the projection of the exact solution onto \mathcal{B}^N , given by (14), and set $U_{i,j,k}^n = U_N^n(x_i, y_j, z_k)$ at a point-wise level. Note that (18) is also

valid. In addition, we have the following truncation error estimates:

$$\begin{split} \frac{\boldsymbol{U}_{N}^{n+1} - \boldsymbol{U}_{N}^{n}}{\Delta t} &= \partial_{t} \boldsymbol{U}_{N} \left(\cdot, t^{n+1/2} \right) + \boldsymbol{\tau}_{2}^{n} (\cdot), \\ \text{with } \left\| \boldsymbol{\tau}_{2} (\cdot) \right\|_{l^{2}(0,T^{*})} &\leq C \Delta t^{2} \| \boldsymbol{U}_{N} (\cdot) \|_{H^{3}(0,T^{*})} \leq C \Delta t^{2}, \\ \frac{3}{2} \boldsymbol{U}_{N}^{n} \cdot \nabla \boldsymbol{U}_{N}^{n} - \frac{1}{2} \boldsymbol{U}_{N}^{n-1} \cdot \nabla \boldsymbol{U}_{N}^{n-1} &= \boldsymbol{U}_{N} \cdot \nabla \boldsymbol{U}_{N} \left(\cdot, t^{n+1/2} \right) + \boldsymbol{\tau}_{3}^{n}, \\ \text{with } \| \boldsymbol{\tau}_{3} \|_{l^{2}(0,T^{*};L^{2})} &\leq C \Delta t^{2} \| \boldsymbol{U}_{N} \|_{H^{2}(0,T^{*};H^{2})}^{2} \leq C \Delta t^{2}, \\ \Delta \left(\frac{3}{4} \boldsymbol{U}_{N}^{n+1} + \frac{1}{4} \boldsymbol{U}_{N}^{n-1} \right) &= \Delta \boldsymbol{U}_{N} \left(\cdot, t^{n+1/2} \right) + \boldsymbol{\tau}_{4}^{n}, \\ \text{with } \| \boldsymbol{\tau}_{4} \|_{l^{2}(0,T^{*};L^{2})} &\leq C \Delta t^{2} \| \boldsymbol{U}_{N} \|_{H^{2}(0,T^{*};H^{2})} \leq C \Delta t^{2}. \end{split}$$

Therefore, the second order consistency of the approximate solution U is established:

$$\frac{U^{n+1} - U^n}{\Delta t} + \frac{3}{2} U^n \cdot \nabla_N U^n - \frac{1}{2} U^{n-1} \cdot \nabla_N U^{n-1} - \nu \Delta_N \left(\frac{3}{4} U^{n+1} + \frac{1}{4} U^{n-1}\right) = \tau^n,$$

with $\tau = I_N(\tau_1 + \tau_2 + \tau_3 + \tau_4), \ \|\tau\|_{l^2(0,T^*;L^2_h)} \le C\left(\Delta t^2 + h^m\right).$ (49)

In other words, the approximate solution satisfies the numerical scheme (47) up to an $O(\Delta t^2 + h^m)$ truncation error. In addition, the H^1 norm of τ is also bounded at the consistency order, namely

$$\|\boldsymbol{\tau}\|_{l^{2}(0,T^{*};H_{h}^{1})} \leq C(\Delta t^{2} + h^{m}).$$
(50)

4.2 Stability and Convergence Analysis

Similar to the first order scheme, the numerical error function is defined by (25) in a pointwise way; u_N^n and e_N^n represent the continuous version of the numerical solution u^n and e^n , respectively. The difference between scheme (47) and the consistency (49) shows that

$$\frac{\boldsymbol{e}^{n+1}-\boldsymbol{e}^n}{\Delta t} + \frac{3}{2} \left(\boldsymbol{e}^n \cdot \nabla_N \boldsymbol{U}^n + \boldsymbol{u}^n \cdot \nabla_N \boldsymbol{e}^n \right) - \frac{1}{2} \left(\boldsymbol{e}^{n-1} \cdot \nabla_N \boldsymbol{U}^{n-1} + \boldsymbol{u}^{n-1} \cdot \nabla_N \boldsymbol{e}^{n-1} \right)$$
$$= \nu \Delta_N \left(\frac{3}{4} \boldsymbol{e}^{n+1} + \frac{1}{4} \boldsymbol{e}^{n-1} \right) + \boldsymbol{\tau}^n.$$
(51)

4.2.1 Leading L^2 Error Estimate

Similarly, the constructed solution U satisfies the $W^{2,\infty}$ regularity condition (27). To deal with a multi-step method, the H^2 a-priori bound is assumed for the numerical error function at all previous time steps:

$$\left\|\boldsymbol{e}_{N}^{k}\right\|_{H^{2}} \leq 1, \quad \text{so that} \left\|\boldsymbol{u}_{N}^{k}\right\|_{H^{2}} \leq \tilde{C}_{0}, \quad \left\|\boldsymbol{u}^{k}\right\|_{\infty} \leq \left\|\boldsymbol{u}_{N}^{k}\right\|_{L^{\infty}} \leq \tilde{C}_{1}, \quad \forall 1 \leq k \leq n, \quad (52)$$

with \tilde{C}_0 , \tilde{C}_1 given by (28)–(29).

Lemma 4 Under the a-priori assumption (52), the numerical error function for the 2nd order scheme (47) satisfies

$$\|\boldsymbol{e}^{n+1}\|_{2} + \sqrt{\frac{1}{2}\nu\Delta t} \sum_{k=1}^{n+1} \|\nabla_{N}\boldsymbol{e}^{k}\|_{2}^{2} \le M_{3}^{2} (\Delta t^{2} + h^{m}).$$
(53)

Proof Taking a discrete L^2 inner product of (51) with $2e^{n+1}$ yields

$$\|\boldsymbol{e}^{n+1}\|_{2}^{2} - \|\boldsymbol{e}^{n}\|_{2}^{2} + \|\boldsymbol{e}^{n+1} - \boldsymbol{e}^{n}\|_{2}^{2} + \nu \Delta t \left\langle \nabla_{N} \left(\frac{3}{2} \boldsymbol{e}^{n+1} + \frac{1}{2} \boldsymbol{e}^{n-1} \right), \nabla_{N} \boldsymbol{e}^{n+1} \right\rangle$$

$$= \Delta t \left\langle \boldsymbol{e}^{n-1} \cdot \nabla_{N} \boldsymbol{U}^{n-1}, \boldsymbol{e}^{n+1} \right\rangle \Delta t \left\langle \boldsymbol{u}^{n-1} \cdot \nabla_{N} \boldsymbol{e}^{n-1}, \boldsymbol{e}^{n+1} \right\rangle$$

$$- 3\Delta t \left\langle \boldsymbol{e}^{n} \cdot \nabla_{N} \boldsymbol{U}^{n}, \boldsymbol{e}^{n+1} \right\rangle - 3\Delta t \left\langle \boldsymbol{u}^{n} \cdot \nabla_{N} \boldsymbol{e}^{n}, \boldsymbol{e}^{n+1} \right\rangle + 2\Delta t \left\langle \boldsymbol{\tau}^{n}, \boldsymbol{e}^{n+1} \right\rangle.$$
(54)

The bound (33) for the truncation error term is also valid. The diffusion term can be analyzed as follows.

$$\left\langle \nabla_{N} \left(\frac{3}{2} \boldsymbol{e}^{n+1} + \frac{1}{2} \boldsymbol{e}^{n-1} \right), \nabla_{N} \boldsymbol{e}^{n+1} \right\rangle = \frac{3}{2} \left\| \nabla_{N} \boldsymbol{e}^{n+1} \right\|_{2}^{2} + \frac{1}{2} \left\langle \nabla_{N} \boldsymbol{e}^{n-1}, \nabla_{N} \boldsymbol{e}^{n+1} \right\rangle$$
$$\geq \frac{3}{2} \left\| \nabla_{N} \boldsymbol{e}^{n+1} \right\|_{2}^{2} - \frac{1}{4} \left\| \nabla_{N} \boldsymbol{e}^{n+1} \right\|_{2}^{2} - \frac{1}{4} \left\| \nabla_{N} \boldsymbol{e}^{n-1} \right\|_{2}^{2}$$
$$\geq \frac{5}{4} \left\| \nabla_{N} \boldsymbol{e}^{n+1} \right\|_{2}^{2} - \frac{1}{4} \left\| \nabla_{N} \boldsymbol{e}^{n-1} \right\|_{2}^{2}. \tag{55}$$

Again, we remark that the key point of the stability analysis for the diffusion term is that the coefficient at time step t^{n+1} dominates the sum of all other diffusion coefficients. The four nonlinear convection terms can be analyzed in a similar way as (35)–(36). The details are skipped.

$$-3\langle \boldsymbol{e}^{n} \cdot \nabla_{N} \boldsymbol{U}^{n}, \boldsymbol{e}^{n+1} \rangle \leq \frac{3}{2} C^{*} (\|\boldsymbol{e}^{n}\|_{2}^{2} + \|\boldsymbol{e}^{n+1}\|_{2}^{2}),$$
(56)

$$\langle \boldsymbol{e}^{n-1} \cdot \nabla_N \boldsymbol{U}^{n-1}, \boldsymbol{e}^{n+1} \rangle \leq \frac{1}{2} C^* (\| \boldsymbol{e}^{n-1} \|_2^2 + \| \boldsymbol{e}^{n+1} \|_2^2),$$
 (57)

$$-3\langle \boldsymbol{u}^{n} \cdot \nabla_{N} \boldsymbol{e}^{n}, \boldsymbol{e}^{n+1} \rangle \leq \frac{1}{4} \nu \| \nabla_{N} \boldsymbol{e}^{n} \|_{2}^{2} + \frac{9\tilde{C}_{1}^{2}}{\nu} \| \boldsymbol{e}^{n+1} \|_{2}^{2},$$
(58)

$$\langle \boldsymbol{u}^{n-1} \cdot \nabla_N \boldsymbol{e}^{n-1}, \boldsymbol{e}^{n+1} \rangle \leq \frac{1}{4} \nu \| \nabla_N \boldsymbol{e}^{n-1} \|_2^2 + \frac{\tilde{C}_1^2}{\nu} \| \boldsymbol{e}^{n+1} \|_2^2.$$
 (59)

Consequently, a substitution of (55), (56), (57), (58), (59) (combined with (33)) into (54) gives

$$\|\boldsymbol{e}^{n+1}\|_{2}^{2} - \|\boldsymbol{e}^{n}\|_{2}^{2} + \frac{5}{4}\nu\Delta t \|\nabla_{N}\boldsymbol{e}^{n+1}\|_{2}^{2} - \frac{1}{4}\nu\Delta t \|\nabla_{N}\boldsymbol{e}^{n}\|_{2}^{2} - \frac{1}{2}\nu\Delta t \|\nabla_{N}\boldsymbol{e}^{n-1}\|_{2}^{2}$$

$$\leq \left(\frac{1\tilde{0}C_{1}^{2}}{\nu} + 2C^{*} + 1\right)\Delta t \|\boldsymbol{e}^{n+1}\|_{2}^{2} + \frac{3}{2}C^{*}\Delta t \|\boldsymbol{e}^{n}\|_{2}^{2} + \frac{1}{2}C^{*}\Delta t \|\boldsymbol{e}^{n-1}\|_{2}^{2} + \Delta t \|\boldsymbol{\tau}^{n}\|_{2}^{2}.$$

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Summing in time gives

$$\|\boldsymbol{e}^{n+1}\|_{2}^{2} + \frac{1}{2}\nu\Delta t\sum_{k=1}^{n+1} \|\nabla_{N}\boldsymbol{e}^{k}\|_{2}^{2} \leq \tilde{C}_{7}\Delta t\sum_{k=0}^{n+1} \|\boldsymbol{e}^{k}\|_{2}^{2} + \Delta t\sum_{k=0}^{n} \|\boldsymbol{\tau}^{n}\|_{2}^{2} + Ch^{2m},$$

with $\tilde{C}_7 = \frac{10\tilde{c}_1^2}{\nu} + 4C^* + 1$. An application of the discrete Gronwall inequality leads to (53), by taking $M_3 = Ce^{\frac{1}{2}\tilde{C}_7T^*}$, with the truncation error estimate (49) used. This in turn gives the $l^{\infty}(0, T^*; L^2) \cap l^2(0, T^*; H^1)$ error estimate for the second order (in time) numerical scheme, under the a-priori H^2 assumption (52).

Similar to the first order scheme, the $l^{\infty}(0, T^*; L^2) \cap l^2(0, T^*; H^1)$ error estimate is not sufficient to recover the a-priori H^2 assumption (52). In the next subsection we will perform an $l^{\infty}(0, T^*; H^2) \cap l^2(0, T^*; H^3)$ error estimate to accomplish it.

4.2.2 Error Estimate in $l^{\infty}(0, T^*; H^2) \cap l^2(0, T^*; H^3)$ Norm

Taking a discrete L^2 inner product of (51) with $2\Delta_N^2 e^{n+1}$ yields

$$\begin{split} \|\Delta_{N}\boldsymbol{e}^{n+1}\|_{2}^{2} &= \|\Delta_{N}\boldsymbol{e}^{n}\|_{2}^{2} + \|\Delta_{N}(\boldsymbol{e}^{n+1}-\boldsymbol{e}^{n})\|_{2}^{2} \\ &+ \nu \Delta t \Big\langle \nabla_{N}\Delta_{N}\Big(\frac{3}{2}\boldsymbol{e}^{n+1} + \frac{1}{2}\boldsymbol{e}^{n-1}\Big), \nabla_{N}\Delta_{N}\boldsymbol{e}^{n+1}\Big\rangle \\ &= \Delta t \left(\big\langle \boldsymbol{e}^{n-1} \cdot \nabla_{N}\boldsymbol{U}^{n-1}, \Delta_{N}^{2}\boldsymbol{e}^{n+1} \big\rangle + \big\langle \boldsymbol{u}^{n-1} \cdot \nabla_{N}\boldsymbol{e}^{n-1}, \Delta_{N}^{2}\boldsymbol{e}^{n+1} \big\rangle \right) \\ &- 3\Delta t \left(\big\langle \boldsymbol{e}^{n} \cdot \nabla_{N}\boldsymbol{U}^{n}, \Delta_{N}^{2}\boldsymbol{e}^{n+1} \big\rangle + \big\langle \boldsymbol{u}^{n} \cdot \nabla_{N}\boldsymbol{e}^{n}, \Delta_{N}^{2}\boldsymbol{e}^{n+1} \big\rangle \right) + 2\Delta t \big\langle \boldsymbol{\tau}^{n}, \Delta_{N}^{2}\boldsymbol{e}^{n+1} \big\rangle. \tag{60}$$

The bound for the truncation error term is the same as (39). The diffusion term can be analyzed similarly to (55):

$$\left\langle \nabla_N \Delta_N \left(\frac{3}{2} \boldsymbol{e}^{n+1} + \frac{1}{2} \boldsymbol{e}^{n-1} \right), \nabla_N \Delta_N \boldsymbol{e}^{n+1} \right\rangle$$

= $\frac{3}{2} \| \nabla_N \Delta_N \boldsymbol{e}^{n+1} \|_2^2 + \frac{1}{2} \langle \nabla_N \Delta_N \boldsymbol{e}^{n-1}, \nabla_N \Delta_N \boldsymbol{e}^{n+1} \rangle$
 $\geq \frac{5}{4} \| \nabla_N \Delta_N \boldsymbol{e}^{n+1} \|_2^2 - \frac{1}{4} \| \nabla_N \Delta_N \boldsymbol{e}^{n-1} \|_2^2.$

The four nonlinear convection terms can be handled in the same fashion as in the first order scheme, with a help of nonlinear expansion in collocation spectral space. We have the following estimates, analogous to (41), (42):

$$-3\langle \boldsymbol{e}^{n} \cdot \nabla_{N} \boldsymbol{U}^{n}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle \leq \frac{1}{8} \nu \| \nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1} \|_{2}^{2} + \frac{864(C^{*})^{2}}{\nu} (\| \nabla_{N} \boldsymbol{e}^{n} \|_{2}^{2} + \| \boldsymbol{e}^{n} \|_{2}^{2}),$$

$$\langle \boldsymbol{e}^{n-1} \cdot \nabla_{N} \boldsymbol{U}^{n-1}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle \leq \frac{1}{8} \nu \| \nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1} \|_{2}^{2} + \frac{96(C^{*})^{2}}{\nu} (\| \nabla_{N} \boldsymbol{e}^{n-1} \|_{2}^{2} + \| \boldsymbol{e}^{n-1} \|_{2}^{2}),$$

$$-3\langle \boldsymbol{u}^{n} \cdot \nabla_{N} \boldsymbol{e}^{n}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle \leq \frac{1}{8} \nu \| \nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1} \|_{2}^{2} + \frac{C\tilde{C}_{1}^{2}}{\nu} \| \Delta_{N} \boldsymbol{e}^{n} \|_{2}^{2},$$

$$\langle \boldsymbol{u}^{n-1} \cdot \nabla_{N} \boldsymbol{e}^{n-1}, \Delta_{N}^{2} \boldsymbol{e}^{n+1} \rangle \leq \frac{1}{8} \nu \| \nabla_{N} \Delta_{N} \boldsymbol{e}^{n+1} \|_{2}^{2} + \frac{C\tilde{C}_{1}^{2}}{\nu} \| \Delta_{N} \boldsymbol{e}^{n-1} \|_{2}^{2}.$$

Going back to (60) results in

$$\begin{split} \|\Delta_{N}\boldsymbol{e}^{n+1}\|_{2}^{2} &- \|\Delta_{N}\boldsymbol{e}^{n}\|_{2}^{2} + \frac{1}{2}\nu\Delta t \|\nabla_{N}\Delta_{N}\boldsymbol{e}^{n+1}\|_{2}^{2} - \frac{1}{4}\nu\Delta t \|\nabla_{N}\Delta_{N}\boldsymbol{e}^{n-1}\|_{2}^{2} \\ &\leq \frac{C(C^{*})^{2}\Delta t}{\nu} (\|\nabla_{N}\boldsymbol{e}^{n}\|_{2}^{2} + \|\nabla_{N}\boldsymbol{e}^{n-1}\|_{2}^{2} + \|\boldsymbol{e}^{n}\|_{2}^{2} + \|\boldsymbol{e}^{n-1}\|_{2}^{2}) \\ &+ \frac{C\tilde{C}_{1}^{2}\Delta t}{\nu} (\|\Delta_{N}\boldsymbol{e}^{n}\|_{2}^{2} + \|\Delta_{N}\boldsymbol{e}^{n-1}\|_{2}^{2}) + \frac{2\Delta t}{\nu} \|\nabla_{N}\boldsymbol{\tau}^{n}\|_{2}^{2}, \\ &\leq \frac{C(\tilde{C}_{1}^{2} + (C^{*})^{2})\Delta t}{\nu} \|\Delta_{N}\boldsymbol{e}^{n}\|_{2}^{2} + \frac{(C(C^{*})^{2}M_{2}^{2} + C)\Delta t}{\nu} (\Delta t^{2} + h^{m})^{2}, \end{split}$$

with the help of the H^1 consistency (50), the leading L^2 convergence (53) and the elliptic regularity. Applying the discrete Gronwall inequality shows that

$$\begin{split} \left\| \Delta_{N} \boldsymbol{e}^{n+1} \right\|_{2}^{2} + \sum_{k=0}^{n} \left\| \Delta_{N} \left(\boldsymbol{e}^{k+1} - \boldsymbol{e}^{k} \right) \right\|_{2}^{2} + \frac{1}{4} \nu \Delta t \sum_{k=1}^{n+1} \left\| \nabla_{N} \Delta_{N} \boldsymbol{e}^{k} \right\|_{2}^{2} \\ & \leq \frac{C((C^{*})^{2} M_{2}^{2} + C)}{\nu} \boldsymbol{e}^{\tilde{c}_{5}T^{*}} \left(\Delta t^{2} + h^{m} \right)^{2} \leq \tilde{C}_{8} \left(\Delta t^{2} + h^{m} \right)^{2}, \end{split}$$

with $\tilde{C}_8 = \frac{C((C^*)^2 M_2^2 + C)}{\nu} e^{\tilde{C}_5 T^*}$. Therefore, the H^2 error estimate for the second order scheme (47) is proven with an application of elliptic regularity:

$$\|\boldsymbol{e}_{N}^{n+1}\|_{H^{2}} \leq C(\|\boldsymbol{e}_{N}^{n+1}\|_{L^{2}} + \|\Delta\boldsymbol{e}_{N}^{n+1}\|_{L^{2}}) \leq \tilde{C}_{9}(\Delta t^{2} + h^{m}), \quad \tilde{C}_{9} = C(M_{2} + \tilde{C}_{8}).$$

Finally, the a-priori H^2 bound (52) for e^{n+1} at time step t^{n+1} can be assured, provided that

$$\Delta t \le (\tilde{C}_9)^{-\frac{1}{2}}, \qquad h \le (\tilde{C}_9)^{-\frac{1}{m}}.$$

This finishes the proof of Theorem 2.

5 Third and Fourth Order Multi-Step Schemes

Similar ideas can be applied to derive third and fourth order in time schemes for (1). The nonlinear convection term is updated by an explicit Adams-Bashforth extrapolation formula, with the time node points t^n , t^{n-1} , ..., t^{n-k+1} involved and an order of accuracy k. The diffusion term is computed by an implicit Adams-Moulton interpolation with the given accuracy order in time. To ensure unconditional numerical stability for a fixed time, we have to derive an Adams-Moulton formula such that the coefficient at time step t^{n+1} dominates the sum of the other diffusion coefficients. In more detail, a k-th order (in time) scheme takes the form of

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t} + \sum_{i=0}^{k-1} B_i \boldsymbol{u}^{n-i} \cdot \nabla_N \boldsymbol{u}^{n-i} = \nu \Delta_N \left(D_0 \boldsymbol{u}^{n+1} + \sum_{i=0}^{k-1} D_{j(i)} \boldsymbol{u}^{n-j(i)} \right).$$
(61)

in which $B_i|_{i=0}^{k-1}$ are the standard Adams-Bashforth coefficients with extrapolation points $t^n, t^{n-1}, \ldots, t^{n-k+1}, j(i)|_{i=0}^{k-1}$ are a set of (distinct) indices with $j(i) \ge 0$, and $D_0, D_{j(i)}|_{i=0}^{k-1}$

correspond to the Adams-Moulton coefficients to achieve the k-th order accuracy. Moreover, a necessary condition for unconditional numerical stability is given by

$$D_0 > \sum_{i=0}^{k-1} \left| D_{j(i)} \right|.$$
(62)

To derive an Adams-Moulton formula for the diffusion term, whose coefficients satisfy the condition (62), we require a stretched stencil. In particular, for the third order scheme, it can be shown that a stencil comprised of the node points t^{n+1} , t^{n-1} and t^{n-3} is adequate. The fully discrete scheme can be formulated as:

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t} + \frac{23}{12} \boldsymbol{u}^n \cdot \nabla_N \boldsymbol{u}^n - \frac{4}{3} \boldsymbol{u}^{n-1} \cdot \nabla_N \boldsymbol{u}^{n-1} + \frac{5}{12} \boldsymbol{u}^{n-2} \cdot \nabla_N \boldsymbol{u}^{n-2} = \nu \Delta_N \left(\frac{2}{3} \boldsymbol{u}^{n+1} + \frac{5}{12} \boldsymbol{u}^{n-1} - \frac{1}{12} \boldsymbol{u}^{n-3} \right).$$
(63)

For the fourth order scheme, we use an Adams-Moulton interpolation at node points t^{n+1} , t^{n-1} , t^{n-5} and t^{n-7} for the diffusion term. Combined with the Adams-Bashforth extrapolation for the nonlinear convection term, the scheme is given by

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t} + \frac{55}{24} \boldsymbol{u}^n \cdot \nabla_N \boldsymbol{u}^n - \frac{59}{24} \boldsymbol{u}^{n-1} \cdot \nabla_N \boldsymbol{u}^{n-1} + \frac{37}{24} \boldsymbol{u}^{n-2} \cdot \nabla_N \boldsymbol{u}^{n-2} - \frac{3}{8} \boldsymbol{u}^{n-3} \cdot \nabla_N \boldsymbol{u}^{n-3} = v \Delta_N \bigg(\frac{757}{1152} \boldsymbol{u}^{n+1} + \frac{470}{1152} \boldsymbol{u}^{n-1} - \frac{118}{1152} \boldsymbol{u}^{n-5} + \frac{43}{1152} \boldsymbol{u}^{n-7} \bigg).$$
(64)

Theorem 3 For any final time $T^* > 0$, assume the exact solution u_e to the 3-D viscous Burgers' equation (1) has a regularity of $H^3(0, T^*; H^{m+3})$ with $m \ge 2$. Denote $u_{\Delta t,h}$ as the continuous (in space) extension of the fully discrete numerical solution given by the third order scheme (63). As $\Delta t, h \to 0$, we have the following convergence result:

$$\|\boldsymbol{u}_{\Delta t,h} - \boldsymbol{u}_{e}\|_{l^{\infty}(0,T^{*};H^{2})} + \sqrt{\nu} \|\boldsymbol{u}_{\Delta t,h} - \boldsymbol{u}_{e}\|_{l^{2}(0,T^{*};H^{3})} \leq C(\Delta t^{3} + h^{m}),$$

provided that the time step Δt and the space grid size h are independently bounded by given constants which depend only on T^* and v.

Proof We look at the approximate solution $U_N(\mathbf{x}, t)$, given by (14), and denote $U_{i,j,k}^n$ as the numerical value of U_N at grid point (x_i, y_j, z_k, t^n) . Again, (18) is satisfied. The following truncation error estimates can be derived using a high order Taylor expansion in time:

$$\begin{split} \boldsymbol{U}_{N}^{n+1} - \boldsymbol{U}_{N}^{n} &= \int_{t^{n}}^{t^{n+1}} \partial_{t} \boldsymbol{U}_{N}(\cdot, t) dt, \\ \frac{23}{12} \boldsymbol{U}_{N}^{n} \cdot \nabla \boldsymbol{U}_{N}^{n} - \frac{4}{3} \boldsymbol{U}_{N}^{n-1} \cdot \nabla \boldsymbol{U}_{N}^{n-1} + \frac{5}{12} \boldsymbol{U}_{N}^{n-2} \cdot \nabla \boldsymbol{U}_{N}^{n-2} = \frac{1}{\Delta t} \int_{t^{n}}^{t^{n+1}} \boldsymbol{U}_{N} \cdot \nabla \boldsymbol{U}_{N}(\cdot, t) dt + \boldsymbol{\tau}_{2}^{n}, \\ \text{with } \|\boldsymbol{\tau}_{2}\|_{l^{2}(0,T^{*};L^{2})} \leq C \Delta t^{3} \|\boldsymbol{U}_{N}\|_{H^{3}(0,T^{*};H^{3})}^{2} \leq C \Delta t^{3}, \\ \Delta \left(\frac{2}{3} \boldsymbol{U}_{N}^{n+1} + \frac{5}{12} \boldsymbol{U}_{N}^{n-1} - \frac{1}{12} \boldsymbol{U}_{N}^{n-3}\right) = \frac{1}{\Delta t} \int_{t^{n}}^{t^{n+1}} \Delta \boldsymbol{U}_{N}(\cdot, t) dt + \boldsymbol{\tau}_{3}^{n}, \end{split}$$

with
$$\|\boldsymbol{\tau}_3\|_{l^2(0,T^*;L^2)} \leq C \Delta t^3 \|\boldsymbol{U}_N\|_{H^3(0,T^*;H^2)} \leq C \Delta t^3$$
.

That in turn leads to the third order consistency of the approximate solution U:

$$\frac{U^{n+1} - U^n}{\Delta t} + \frac{23}{12} U^n \cdot \nabla_N U^n - \frac{4}{3} U^{n-1} \cdot \nabla_N U^{n-1} + \frac{5}{12} U^{n-2} \cdot \nabla_N U^{n-2} - \nu \Delta_N \left(\frac{2}{3} U^{n+1} + \frac{5}{12} U^{n-1} - \frac{1}{12} U^{n-3}\right) = \boldsymbol{\tau}^n,$$
(65)

with $\|\boldsymbol{\tau}\|_{l^2(0,T^*;L^2_h)} \leq C(\Delta t^3 + h^m)$. The H^1 bound of $\boldsymbol{\tau}$ can also be derived:

$$\|\boldsymbol{\tau}\|_{l^2(0,T^*;H_h^1)} \leq C(\Delta t^3 + h^m).$$

Subsequently, with the numerical error function denoted by (25) (while e_N^n represents the continuous version of e^n), the difference between (63) and (65) gives

$$\frac{e^{n+1} - e^n}{\Delta t} + \frac{23}{12} (e^n \cdot \nabla_N U^n + u^n \cdot \nabla_N e^n) - \frac{4}{3} (e^{n-1} \cdot \nabla_N U^{n-1} + u^{n-1} \cdot \nabla_N e^{n-1}) + \frac{5}{12} (e^{n-2} \cdot \nabla_N U^{n-2} + u^{n-2} \cdot \nabla_N e^{n-2}) = v \Delta_N \left(\frac{2}{3} e^{n+1} + \frac{5}{12} e^{n-1} - \frac{1}{12} e^{n-3} \right) + \tau^n.$$
(66)

Similar to the analysis of the second order scheme, we make the H^2 a-priori assumption (52) for the numerical error function at all previous time steps. Taking a discrete L^2 inner product of (66) with $2e^{n+1}$ yields

$$\|\boldsymbol{e}^{n+1}\|_{2}^{2} - \|\boldsymbol{e}^{n}\|_{2}^{2} + \|\boldsymbol{e}^{n+1} - \boldsymbol{e}^{n}\|_{2}^{2} + \nu \Delta t \left\langle \nabla_{N} \left(\frac{4}{3}\boldsymbol{e}^{n+1} + \frac{5}{6}\boldsymbol{e}^{n-1} - \frac{1}{6}\boldsymbol{e}^{n-3}\right), \nabla_{N}\boldsymbol{e}^{n+1} \right\rangle$$

$$= \frac{8}{3} \Delta t \left\langle \boldsymbol{e}^{n-1} \cdot \nabla_{N} \boldsymbol{U}^{n-1}, \boldsymbol{e}^{n+1} \right\rangle + \frac{8}{3} \Delta t \left\langle \boldsymbol{u}^{n-1} \cdot \nabla_{N} \boldsymbol{e}^{n-1}, \boldsymbol{e}^{n+1} \right\rangle$$

$$- \frac{5}{6} \Delta t \left\langle \boldsymbol{e}^{n-2} \cdot \nabla_{N} \boldsymbol{U}^{n-2}, \boldsymbol{e}^{n+1} \right\rangle - \frac{5}{6} \Delta t \left\langle \boldsymbol{u}^{n-2} \cdot \nabla_{N} \boldsymbol{e}^{n-2}, \boldsymbol{e}^{n+1} \right\rangle$$

$$- \frac{23}{6} \Delta t \left\langle \boldsymbol{e}^{n} \cdot \nabla_{N} \boldsymbol{U}^{n}, \boldsymbol{e}^{n+1} \right\rangle - \frac{23}{6} \Delta t \left\langle \boldsymbol{u}^{n} \cdot \nabla_{N} \boldsymbol{e}^{n}, \boldsymbol{e}^{n+1} \right\rangle + 2 \Delta t \left\langle \boldsymbol{\tau}^{n}, \boldsymbol{e}^{n+1} \right\rangle. \tag{67}$$

Since the diffusion coefficient at t^{n+1} dominates the other ones, the viscosity term can be analyzed in the same way as (55):

$$\left\langle \nabla_{N} \left(\frac{4}{3} e^{n+1} + \frac{5}{6} e^{n-1} - \frac{1}{6} e^{n-3} \right), \nabla_{N} e^{n+1} \right\rangle$$

= $\frac{4}{3} \| \nabla_{N} e^{n+1} \|_{2}^{2} + \frac{5}{6} \langle \nabla_{N} e^{n-1}, \nabla_{N} e^{n+1} \rangle - \frac{1}{6} \langle \nabla_{N} e^{n-3}, \nabla_{N} e^{n+1} \rangle$
\ge $\frac{5}{6} \| \nabla_{N} e^{n+1} \|_{2}^{2} - \frac{5}{12} \| \nabla_{N} e^{n-1} \|_{2}^{2} - \frac{1}{12} \| \nabla_{N} e^{n-3} \|_{2}^{2}.$

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The estimates for the nonlinear convection terms are given below. The details are skipped.

$$\begin{aligned} &-\frac{23}{6} \langle \boldsymbol{e}^{n} \cdot \nabla_{N} \boldsymbol{U}^{n}, \boldsymbol{e}^{n+1} \rangle + \frac{8}{3} \langle \boldsymbol{e}^{n-1} \cdot \nabla_{N} \boldsymbol{U}^{n-1}, \boldsymbol{e}^{n+1} \rangle - \frac{5}{6} \langle \boldsymbol{e}^{n-2} \cdot \nabla_{N} \boldsymbol{U}^{n-2}, \boldsymbol{e}^{n+1} \rangle \\ &\leq \frac{11}{3} C^{*} \left(\left\| \boldsymbol{e}^{n+1} \right\|_{2}^{2} + \left\| \boldsymbol{e}^{n} \right\|_{2}^{2} + \left\| \boldsymbol{e}^{n-1} \right\|_{2}^{2} + \left\| \boldsymbol{e}^{n-2} \right\|_{2}^{2} \right), \\ &- \frac{23}{6} \langle \boldsymbol{u}^{n} \cdot \nabla_{N} \boldsymbol{e}^{n}, \boldsymbol{e}^{n+1} \rangle + \frac{8}{3} \langle \boldsymbol{u}^{n-1} \cdot \nabla_{N} \boldsymbol{e}^{n-1}, \boldsymbol{e}^{n+1} \rangle - \frac{5}{6} \langle \boldsymbol{u}^{n-2} \cdot \nabla_{N} \boldsymbol{e}^{n-2}, \boldsymbol{e}^{n+1} \rangle \\ &\leq \frac{1}{12} \nu \left(\left\| \nabla_{N} \boldsymbol{e}^{n} \right\|_{2}^{2} + \left\| \nabla_{N} \boldsymbol{e}^{n-1} \right\|_{2}^{2} + \left\| \nabla_{N} \boldsymbol{e}^{n-2} \right\|_{2}^{2} \right) + \frac{C \tilde{C}_{1}^{2}}{\nu} \left\| \boldsymbol{e}^{n+1} \right\|_{2}^{2}. \end{aligned}$$

Going back to (67) results in

$$\begin{aligned} \|\boldsymbol{e}^{n+1}\|_{2}^{2} &- \|\boldsymbol{e}^{n}\|_{2}^{2} + \frac{5}{6}\nu\Delta t \|\nabla_{N}\boldsymbol{e}^{n+1}\|_{2}^{2} - \frac{1}{12}\nu\Delta t \|\nabla_{N}\boldsymbol{e}^{n}\|_{2}^{2} - \frac{1}{2}\nu\Delta t \|\nabla_{N}\boldsymbol{e}^{n-1}\|_{2}^{2} \\ &- \frac{1}{12}\nu\Delta t (\|\nabla_{N}\boldsymbol{e}^{n-2}\|_{2}^{2} + \|\nabla_{N}\boldsymbol{e}^{n-3}\|_{2}^{2}) \\ &\leq \left(\frac{C\tilde{C}_{1}^{2}}{\nu} + CC^{*} + C\right)\Delta t \|\boldsymbol{e}^{n+1}\|_{2}^{2} + CC^{*}\Delta t (\|\boldsymbol{e}^{n}\|_{2}^{2} + \|\boldsymbol{e}^{n-1}\|_{2}^{2} + \|\boldsymbol{e}^{n-2}\|_{2}^{2}) + \Delta t \|\boldsymbol{\tau}^{n}\|_{2}^{2}. \end{aligned}$$

Consequently, summing in time, applying the discrete Gronwall inequality and using a simple fact that $\frac{5}{6} - \frac{3}{12} - \frac{1}{2} = \frac{1}{12} > 0$, we get a fixed time $O(\Delta t^3 + h^m)$ convergence for the third order scheme (63) in $L^{\infty}(0, T^*; L^2)$ norm:

$$\|\boldsymbol{e}^{n+1}\|_{2}^{2} + \frac{1}{12}\nu\Delta t\sum_{k=1}^{n+1} \|\nabla_{N}\boldsymbol{e}^{k}\|_{2}^{2} \leq \tilde{C}_{10}(\Delta t^{3} + h^{m})^{2},$$

under the a-priori $H^{\frac{3}{2}+\delta}$ assumption (52).

Similar convergence analysis in $L^{\infty}(0, T^*; H^2) \cap L^2(0, T^*; H^3)$ can be performed by taking a discrete L^2 inner product of (66) with $2\Delta_N^2 e^{n+1}$. The details are skipped.

$$\|\Delta_{N}\boldsymbol{e}^{n+1}\|_{2}^{2} + \sum_{k=0}^{n} \|\Delta_{N}(\boldsymbol{e}^{k+1} - \boldsymbol{e}^{k})\|_{2}^{2} + \frac{1}{24}\nu\Delta t \sum_{k=1}^{n+1} \|\nabla_{N}\Delta_{N}\boldsymbol{e}^{k}\|_{2}^{2} \leq \tilde{C}_{11}(\Delta t^{3} + h^{m})^{2};$$

hence,

$$\|\boldsymbol{e}_{N}^{n+1}\|_{H^{2}} \leq C(\|\boldsymbol{e}_{N}^{n+1}\|_{L^{2}} + \|\Delta\boldsymbol{e}_{N}^{n+1}\|_{L^{2}}) \leq \tilde{C}_{12}(\Delta t^{3} + h^{m}), \quad \tilde{C}_{12} = C\sqrt{\tilde{C}_{10} + \tilde{C}_{11}}.$$

Finally, the a-priori H^2 bound (52) for e^{n+1} at time step t^{n+1} is assured, provided that

$$\Delta t \le (\tilde{C}_{12})^{-\frac{1}{3}}, \qquad h \le (\tilde{C}_{12})^{-\frac{1}{m}}.$$

Remark 5 For the second order in time method, treating the diffusion term with a standard second order Adams-Moulton formula leads to a Crank-Nicolson scheme. In the third order case, we observe that a direct application of the Adams-Moulton formula at the nodes t^{n+1} , t^n and t^{n-1} (corresponding to j(i) = i in the general form (61)) does not give a formula

with the stated stability property. For example, a "naive" combination of 3rd order Adams-Bashforth for the nonlinear convection and Adams-Moulton for the diffusion term results in the following scheme

$$\frac{\boldsymbol{u}^{n+1}-\boldsymbol{u}^n}{\Delta t} + \frac{23}{12}\boldsymbol{u}^n \cdot \nabla_N \boldsymbol{u}^n - \frac{4}{3}\boldsymbol{u}^{n-1} \cdot \nabla_N \boldsymbol{u}^{n-1} + \frac{5}{12}\boldsymbol{u}^{n-2} \cdot \nabla_N \boldsymbol{u}^{n-2} \\ = \boldsymbol{v} \Delta_N \bigg(\frac{5}{12} \boldsymbol{u}^{n+1} + \frac{2}{3} \boldsymbol{u}^n - \frac{1}{12} \boldsymbol{u}^{n-1} \bigg),$$

which violates the stability condition (62). Numerical experiments also showed that this method is unstable in time. This case highlights the need to choose an appropriate time-discretization to couple with the pseudospectral method.

Remark 6 There have been extensive numerical simulation works of high-order multi-step, semi-implicit schemes applied to nonlinear time-dependent PDEs. Among them, it is worth mentioning the AB/BDI (Adams-Bashforth/Implicit Backward Differentiation) schemes, introduced by Crouzeix [10], which update the nonlinear convection term using the standard Adams-Bashforth extrapolation and the time marching term with implicit backward differentiation for the diffusion term. In particular, the third order scheme of this family has been applied to the incompressible Navier-Stokes equations with various spatial approximations; see the relevant works [2, 3, 23, 26]. However, only the linear stability analysis is covered in these existing works; see the relevant discussions in [36]. To the authors' knowledge, this article is the first to provide the stability and convergence analysis for a third order scheme applied to nonlinear PDE.

The stability and convergence for the fourth order scheme (64) with a fixed final time is given in the following theorem.

Theorem 4 For any final time $T^* > 0$, assume the exact solution u_e to the 3-D viscous Burgers' equation (1) has a regularity of $H^4(0, T^*; H^{m+3})$ with $m \ge 2$. Denote $u_{\Delta t,h}$ as the continuous (in space) extension of the fully discrete numerical solution given by the fourth order scheme (64). As $\Delta t, h \to 0$, we have the following convergence result:

$$\|\boldsymbol{u}_{\Delta t,h} - \boldsymbol{u}_e\|_{l^{\infty}(0,T^*;H^2)} + \sqrt{\nu} \|\boldsymbol{u}_{\Delta t,h} - \boldsymbol{u}_e\|_{l^{2}(0,T^*;H^3)} \le C(\Delta t^4 + h^m),$$

provided that the time step Δt and the space grid size h are independently bounded by given constants which only depend on T^* and v.

We omit the full proof of this theorem because of its similarity with the previous proofs. However, we detail the estimate of the diffusion term for the fourth order scheme (64):

$$\left\langle \nabla_{N} \left(\frac{757}{1152} e^{n+1} + \frac{470}{1152} e^{n-1} - \frac{118}{1152} e^{n-5} + \frac{43}{1152} e^{n-7} \right), \nabla_{N} e^{n+1} \right\rangle$$

$$= \frac{757}{1152} \left\| \nabla_{N} e^{n+1} \right\|_{2}^{2} + \frac{470}{1152} \langle \nabla_{N} e^{n-1}, \nabla_{N} e^{n+1} \rangle - \frac{118}{1152} \langle \nabla_{N} e^{n-5}, \nabla_{N} e^{n+1} \rangle$$

$$+ \frac{43}{1152} \langle \nabla_{N} e^{n-7}, \nabla_{N} e^{n+1} \rangle$$

$$\geq \frac{883}{2304} \left\| \nabla_{N} e^{n+1} \right\|_{2}^{2} - \frac{470}{2304} \left\| \nabla_{N} e^{n-1} \right\|_{2}^{2} - \frac{118}{2304} \left\| \nabla_{N} e^{n-5} \right\|_{2}^{2} - \frac{43}{2304} \left\| \nabla_{N} e^{n-5} \right\|_{2}^{2}.$$

Again, the fact that the diffusion coefficient at t^{n+1} dominates the other ones, i.e., $\frac{883}{2304} - \frac{470}{2304} - \frac{118}{2304} - \frac{43}{2304} = \frac{252}{2304} > 0$, ensures the numerical stability of (64).

6 Conclusions

In this paper we develop stable time-stepping methods of order up to four for the numerical solution of the three dimensional viscous Burgers' equation by a Fourier collocation method, and present a novel stability and convergence analysis for the fully discrete methods.

In the first order (in time) scheme, we apply a semi-implicit approach, which updates the nonlinear convection term explicitly and treats the diffusion term implicitly. Since the pseudospectral method is evaluated at the interpolation grid points, a discrete L^2 and H^m inner product is used to carry out the analysis. The stability analysis requires an estimate of the nonlinear convection term in the L^2 and H^1 norms. This estimate cannot be obtained directly, due to the aliasing error complicated by the nonlinearity. A key observation of this article is that, if the nonlinearity is of polynomial type (for example, quadratic for Burgers' equation or the Navier-Stokes equations), the corresponding interpolation operator applied to the nonlinear expansion results in an L^2 or any H^k norm bounded by a given constant multiple of the corresponding norms of the original exact nonlinear term; see Lemma 1. As a result, all the energy estimates in the Sobolev norms can be performed almost in the same way as in the Galerkin approach, so that stability and convergence over a fixed finite time is demonstrated.

The L^{∞} bound of the numerical solution is the key point in the stability and convergence analysis of a fully discrete scheme for nonlinear PDEs. The classical way to obtain such a bound is the application of the inverse inequality which provides an L^{∞} bound of the numerical solution after the L^2 numerical convergence is established. However, this approach leads to a restriction on the time-step in terms of the spatial grid size, which can be prohibitive in two or three dimensions. In this work, we avoid the inverse inequality approach. Instead, we provide an H^2 error estimate so that the L^{∞} norm of the numerical solution is automatically bounded, using a 3-D Sobolev embedding. This approach avoids a time-step restriction in terms of the spatial grid size.

We apply similar ideas to develop stable higher order in time schemes using a multistep approach. For the sake of numerical efficiency, the semi-implicit pattern is kept, with a standard Adams-Bashforth extrapolation formula (with the given accuracy) applied to the nonlinear term, while the diffusion term is treated using an implicit Adams-Moulton interpolation formula on certain time node points. However, deriving a stable scheme requires specialized stretched stencil in the Adams-Moulton approximation. We present these multistep schemes with accuracy up to fourth order and show that, coupled with the Fourier collocation method, these methods are stable and convergent.

References

- 1. Abia, L., Sanz-Serna, J.M.: The spectral accuracy of a fully-discrete scheme for a nonlinear third order equation. Computing **44**, 187–196 (1990)
- Botella, O.: On the solution of the Navier-Stokes equations using projection schemes with third-order accuracy in time. Comput. Fluids 26, 107–116 (1997)
- Botella, O., Peyret, R.: Computing singular solutions of the Navier-Stokes equations with the Chebyshevcollocation method. Int. J. Numer. Methods Fluids 36, 125–163 (2001)
- 4. Boyd, J.: Chebyshev and Fourier Spectrum Methods, 2nd edn. Dover, New York (2001)

- Bressan, A., Quarteroni, A.: An implicit/explicit spectral method for Burgers' equation. Calcolo 23(3), 265–284 (1986)
- Canuto, C., Quarteroni, A.: Approximation results for orthogonal polynomials in Sobolev spaces. Math. Comput. 38, 67–86 (1982)
- Canuto, C., Hussani, M.Y., Quarteroni, A., Zang, T.A.: Spectral Methods: Fundamentals in Single Domains. Springer, Berlin (2006)
- Canuto, C., Hussani, M.Y., Quarteroni, A., Zang, T.A.: Spectral Methods: Evolution to Complex Geometries and Applications to Fluid Dynamics. Springer, Berlin (2007)
- Chen, G.Q., Du, Q., Tadmor, E.: Super viscosity approximations to multi-dimensional scalar conservation laws. Math. Comput. 61(204), 629–643 (1993)
- Crouzeix, M.: Une methode multipas implicite-explicite pour l'approximation des'equations d'evolution paraboliques. Numer. Math. 35, 257–276 (1982)
- De Frutos, J., Ortega, T., Sanz-Serna, J.M.: Pseudo-spectral method for the "Good" Boussinesq equation. Math. Comput. 57(195), 109–122 (1991)
- Du, Q., Guo, B., Shen, J.: Fourier spectral approximation to a dissipative system modeling the flow of liquid crystals. SIAM J. Numer. Anal. 39(3), 735–762 (2001)
- Faure, S., Laminie, J., Temam, R.: Finite volume discretization and multilevel methods in flow problems. J. Sci. Comput. 25(112), 231–261 (2005)
- Gottlieb, D., Orszag, S.A.: Numerical Analysis of Spectral Methods, Theory and Applications. SIAM, Philadelphia (1977)
- Gottlieb, D., Temam, R.: Implementation of the nonlinear Galerkin method with pseudospectral (collocation) discretizations. Appl. Numer. Math. 12, 119–134 (1993)
- Guo, B.Y.: A spectral method for the vorticity equation on the surface. Math. Comput. 64(211), 1067– 1069 (1995)
- Guo, B.Y., Huang, W.: Mixed Jacobi-spherical harmonic spectral method for Navier–Stokes equations. Appl. Numer. Math. 57(8), 939–961 (2007)
- Guo, B.Y., Shen, J.: On spectral approximations using modified Legendre rational functions: application to the Korteweg-de Vries equation on the half line. Indiana Univ. Math. J. 50, 181–204 (2001). Special issue: Dedicated to Professors Ciprian Foias and Roger Temam
- Guo, B.Y., Zou, J.: Fourier spectral projection method and nonlinear convergence analysis for Navier-Stokes equations. J. Math. Anal. Appl. 282(2), 766–791 (2003)
- Guo, B.Y., Li, J., Ma, H.P.: Fourier-Chebyshev spectral method for solving three-dimensional vorticity equation. Acta Math. Appl. Sin. 11(1), 94–109 (1995)
- Guo, B.Y., Ma, H.P., Tadmor, E.: Spectral vanishing viscosity method for nonlinear conservation laws. SIAM J. Numer. Anal. 39, 1254–1268 (2001)
- Hesthaven, J., Gottlieb, S., Gottlieb, D.: Spectral Methods for Time-Dependent Problems. Cambridge University Press, Cambridge (2007)
- Karniadakis, G., Israeli, M., Orszag, S.: High-order splitting methods for the incompressible Navier-Stokes equations. J. Comput. Phys. 97, 414–443 (1991)
- Kreiss, H.O., Oliger, J.: Methods for Approximate Solution of Time-Dependent Problems. GARP Publications, vol. 10. World Meteorological Organization, Geneva (1973)
- Ladyzhenskaya, O.A., Solonnikov, V.A., Ural'ceva, N.N.: Linear and Quasi-Linear Equations of Parabolic Type. AMS, Providence (1967)
- Le Quere, P.: Transition to unsteady natural convection in a tall water-filled cavity. Phys. Fluids A 2, 503–515 (1990)
- Liu, C., Shen, J.: A phase field model for the mixture of two incompressible fluids and its approximation by a Fourier-spectral method. Physica D 179, 211–228 (2003)
- Ma, H.P.: Chebyshev-Legendre super spectral viscosity method for nonlinear conservation laws. SIAM J. Numer. Anal. 35, 893–908 (1998)
- Maday, Y., Quarteroni, A.: Legendre and Chebyshev spectral approximations of Burgers' equation. Numer. Math. 37, 321–332 (1981)
- Maday, Y., Quarteroni, A.: Approximation of Burgers' equation by pseudospectral methods. RAIRO. Anal. Numér. 16, 375–404 (1982)
- Maday, Y., Quarteroni, A.: Spectral and pseudospectral approximation to Navier-Stokes equations. SIAM J. Numer. Anal. 19(4), 761–780 (1982)
- Maday, Y., Ould Kaber, S.M., Tadmor, E.: Legendre pseudospectral viscosity method for nonlinear conservation laws. SIAM J. Numer. Anal. 30(2), 321–342 (1993)
- Majda, A., McDonough, J., Osher, S.: The Fourier method for non-smooth initial data. Math. Comput. 32, 1041–1081 (1978)
- 34. Marion, M., Temam, R.: Nonlinear Galerkin methods. SIAM J. Numer. Anal. 26, 1139–1157 (1989)

- Marion, M., Temam, R.: Nonlinear Galerkin methods: the finite element case. Numer. Math. 57, 205–226 (1990)
- 36. Peyret, R.: Spectral Methods for Incompressible Viscous Flow. Springer, New York (2001)
- Shen, J., Temam, R.: Nonlinear Galerkin method using Chebyshev and Legendre polynomials I. The one-dimensional case. SIAM J. Numer. Anal. 32, 215–234 (1995)
- Tadmor, E.: The exponential accuracy of Fourier and Chebyshev differencing methods. SIAM J. Numer. Anal. 23, 1–10 (1986)
- Tadmor, E.: Convergence of spectral methods to nonlinear conservation laws. SIAM J. Numer. Anal. 26(1), 30–44 (1989)
- Tadmor, E.: Shock capturing by the spectral viscosity method. Comput. Methods Appl. Mech. Eng. 80, 197–208 (1990)
- Tadmor, E.: Total variation and error estimates for spectral viscosity approximations. Math. Comput. 60(201), 245–256 (1993)
- 42. Tadmor, E.: Burgers' equation with vanishing hyper-viscosity. Commun. Math. Sci. 2(2), 317–324 (2004)
- 43. Temam, R.: Navier-Stokes Equations: Theory and Numerical Analysis. AMS, Providence (2001)
- Weinan, E.: Convergence of spectral methods for the Burgers' equation. SIAM J. Numer. Anal. 29(6), 1520–1541 (1992)
- Weinan, E.: Convergence of Fourier methods for Navier-Stokes equations. SIAM J. Numer. Anal. 30(3), 650–674 (1993)
- Wu, S., Liu, X.: Convergence of spectral method in time for the Burgers' equation. Acta Math. Appl. Sin. 13(3), 314–320 (1997)