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NONLINEAR MODEL REDUCTION USING GROUP PROPER ORTHOGONAL DECOMPOSITION

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Abstract. We propose a new method to reduce the cost of computing nonlinear terms in projection based reduced order models with global basis functions. We develop this method by extending ideas from the group finite element (GFE) method to proper orthogonal decomposition (POD) and call it the group POD method. Here, a scalar two-dimensional Burgers' equation is used as a model problem for the group POD method. Numerical results show that group POD models of Burgers' equation are as accurate and are computationally more efficient than standard POD models of Burgers' equation.

Key words. model reduction, proper orthogonal decomposition, group finite element, nonlinear

1. Introduction

A challenge in the simulation of systems modeled by partial differential equations (PDE) is to reduce computational cost while preserving accuracy. To this end, much research in numerous aspects of the simulation of PDE has been performed. These efforts include attempts to reduce computational cost by improving algorithmic efficiency, developing parallel computing schemes, and applying model order reduction techniques. For example, reduced order modeling for fluid flows has seen extensive application of the Galerkin projection with proper orthogonal decomposition (POD) [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11].

In this work, we submit a new method to reduce the cost of computing nonlinear terms in projection based reduced order models with global basis functions by extending ideas from the group finite element (GFE) method to POD[1]. We shall further refer to this approach as the group proper orthogonal decomposition (POD) method.

The GFE method, also known as product approximation, expresses the nonlinear terms of a PDE in grouped form - as the product of separate space and time dependent quantities. This leads to the spatial discretization of nonlinear terms being computed *once* before integration and a substantial reduction in computational cost [12, 13, 14]. Here, instead of projecting grouped nonlinear terms onto a local finite element basis, we show that the projection of grouped nonlinear terms onto a set of global basis functions reduces the cost of simulation due to symmetry in the nonlinear terms. Although a Galerkin projection onto a POD basis is used here for illustration, we anticipate this method to be generally applicable to other global basis functions and Petrov-Galerkin projections.

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[1]We note that this method has also been independently investigated by Max Gunzburger (private communication).

To determine the accuracy of the group POD method, computational solutions of group POD and standard POD models of Burgers' equation are compared to analytical manufactured benchmark solutions [15, 16, 17, 18, 19]. Our experiments show close agreement between simulations of the group POD and standard POD models of Burgers' equation.

To assess the computational cost of the group POD method, total integration times and operation counts for the nonlinear terms of the group POD model of Burgers' equation are compared to the standard POD model. For the quadratic nonlinearity of Burgers' equation, our results show the group POD method provides a clear computational advantage over the standard POD approach in terms of operation count and total integration time.

Following this introduction, we provide background on POD and the GFE method. The standard and group POD models of Burgers' equation are developed in Section 3, followed by their implementation and operation counts in Section 4. Section 5 contains numerical results which demonstrates that group POD models of Burgers' equation are as accurate and are more efficient than the standard POD form. Finally, we provide a mathematical extension of the group POD method to cubic nonlinearities in Section 6.

2. Background

We begin by providing background on two concepts key to the group POD method: proper orthogonal decomposition (POD) itself and the group finite element (GFE) method. While POD offers computational advantages through a reduction in order, the GFE method offers computational gains through the construction of nonlinear terms. Following the background on POD, we illustrate the computational advantage of grouping the nonlinear terms with the GFE form of Burgers' equation.

2.1. Notation. To describe POD based model reduction for partial differential equations, we use the following notation. Let X be a Hilbert space with its inner product and corresponding norm denoted $(\cdot,\cdot)_X$ and $\|\cdot\|_X$, respectively. A function, u, is in $L^2(0,T;X)$ if for each $0 \le t \le T$, $u(t)$ is in X, and $\int_0^T \|u(t)\|_X^2\, dt < \infty$.

2.2. Proper Orthogonal Decomposition (POD). At the turn of the twentieth century, the closest fitting lines or planes to a set of points in space was investigated by Pearson [20]. Independently, almost three decades later, a similar treatment appeared by Hotelling where the "method of principal components" was coined [21]. The analysis presented in [20] and [21] formed the linear algebraic approach to what many now call proper orthogonal decomposition (POD).

Since the work of Pearson and Hotelling, many have studied or used POD in a range of fields such as oceanography [22], fluid mechanics [1, 2, 4], system feedback control [23, 24, 25, 26, 27, 28], and system modeling [5, 8, 10, 29]. Following many predecessors, we use POD as tool for model reduction where the POD of a function, $u \in L^2(0,\infty;X)$, gives a basis that best represents $u \in L^2(0,\infty;X)$ in a mean-square sense [8, 9].

The method of snapshots is a practical approach to compute the POD of a function known pointwise in time. The method of snapshots may be derived from the continuous POD operator by assuming a piecewise constant representation of u in time as shown in [9]. The remainder of this section outlines the procedure.

Suppose $u \in L^2(0,T;X)$ is obtained at times $t_1 < t_2 < t_3 \ldots < t_S$ such that $t_i \in [0,T]$ for $i = 1,\ldots,S$, and the value of the time step size, $\triangle t = t_{i+1} - t_i$, for $i = 1,\ldots,(S-1)$, is constant. Let the set $\{u(t_i)\}_{i=1}^S$ denote the set of S snapshots of a solution, $u(t)$, of a dynamic system. Then, the correlation matrix, $\mathbf{K}$, of the data set $\{u(t_i)\}_{i=1}^S$ may be defined as

$$\mathbf{K} = \left(\frac{1}{S}(u_i, u_j)_X\right)_{i,j=1}^S \tag{1}$$

where $u_i = u(t_i)$ and $u_j = u(t_j)$ are the ith and jth snapshot of $u(t)$. Let $\{\lambda_k, v_k\}$ denote the eigenvalues of $\mathbf{K}$ and the corresponding normalized eigenvectors. Then, the kth POD basis function of the POD basis set $\Psi = \{\psi_k\}_{k=1}^S$ is given by

$$\psi_k = \frac{1}{\sqrt{S\,\lambda_k}} \sum_{i=1}^{S} [v_k]_i u_i, \tag{2}$$

where $[v_k]_i$ represents the ith element of the kth orthonormal eigenvector of $\mathbf{K}$.

Note that ψ_k, computed from equation (2), shares the same representation as the snapshot set $\{u_i\}_{i=1}^S$. For example, if each snapshot is represented as

$$u_i = \sum_{\ell=1}^{N} R_\ell(t_i)\beta_\ell(\mathbf{x})$$

where each $R_\ell(t_i)$ is a time dependent coefficient, and $\{\beta_\ell(\mathbf{x})\}$ is a collection of functions; it follows that the kth POD mode $\psi_k(\mathbf{x})$ is given by

$$\psi_k(\mathbf{x}) = \sum_{\ell=1}^{N} \gamma_{\ell k}\beta_\ell(\mathbf{x}) \tag{3}$$

where the coefficients $\gamma_{\ell k}$ are computed from (2) as

$$\gamma_{\ell k} = \frac{1}{\sqrt{S\,\lambda_k}} \sum_{i=1}^{S} [v_k]_i R_\ell(t_i).$$

The general representation of the POD mode (3) will be used in Section 4 in the implementation of the group and standard POD models of Burgers' equation.

2.3. The Group Finite Element (GFE) Method. The group finite element (GFE) method, also known as "product approximation," is a finite element (FE) technique for certain types of nonlinear partial differential equations. Experiments with the GFE method have shown an increase in economy and a slight increase in the nodal accuracy compared to FE solutions of the unsteady Burgers' equations and many other problems [12, 13, 14]. The authors are unaware of convergence theory for the GFE applied to Burgers' equation; however, theoretical results exist for other problems [12, 30, 31, 32, 33, 34, 35]

Here, we illustrate the GFE method with its application to a model problem. Consider the following form of Burgers' equation

$$
\begin{aligned}
& u_t + uu_x + uu_y - \nu\,(\nabla^2 u) \;=\; f, \qquad (x,y) \in \Omega, \qquad t > 0, \\
& u(t, \partial\Omega) = 0, \qquad t > 0, \\
& u(0,x,y) = u_0(x,y), \qquad (x,y) \in \Omega\,,
\end{aligned}
\tag{4}
$$

where $u = u(t,x,y) = u(t,\mathbf{x})$ represents the dependent variable, $f = f(t,x,y)$ is some forcing on the system, ν is a constant positive parameter, and $\partial\Omega$ denotes the boundary of the spatial domain, Ω.

The GFE method requires two main steps: rewriting the nonlinear terms of the governing equations in grouped form and determining a supplementary grouped trial function. The nonlinear terms of Burgers' equation (4) may be grouped as

$$
uu_x + uu_y = \frac{1}{2}(u^2)_x + \frac{1}{2}(u^2)_y,
\tag{5}
$$

so that the grouped variable, u^2, is identified. Let a standard FE approximation to $u(t,\mathbf{x})$ be written

$$
u(t,\mathbf{x}) \approx u_N(t,\mathbf{x}) = \sum_{j=1}^{N} \alpha_j(t)\beta_j(\mathbf{x}),
\tag{6}
$$

where N is the number of basis functions, $\beta_j(\mathbf{x})$ is the jth piecewise linear FE basis function, and each $\alpha_j(t)$ is an undetermined function of time. In the group method, the FE trial function is required to interpolate the grouped variable, u^2, at the nodes, that is,

$$
u^2(t,\mathbf{x}_n) \approx u_N^2(t,\mathbf{x}_n) = \left[\sum_{j=1}^{N} \alpha_j(t)\beta_j(\mathbf{x}_n)\right]^2,
\tag{7}
$$

where $\mathbf{x}_n = (x_n, y_n)$ is the nth node point of a computational grid. Note that at the nodes

$$
\beta_j(\mathbf{x}_n) = \begin{cases} 1 & \text{if} \quad j = n \\ 0 & \text{if} \quad j \neq n \end{cases},
$$

since the basis is piecewise linear. Thus, the right hand side of (7) may be simplified to give the group finite element approximation at the nodes

$$
u_N^2(t,\mathbf{x}_n) = \sum_{j=1}^{N} \alpha_j^2(t)\beta_j(\mathbf{x}_n).
\tag{8}
$$

Let Q_X denote the operator that maps the nodal approximation (8) onto its piecewise linear interpolant. Then, the grouped approximation may be represented continuously over the entire domain as

$$
u_N^2(t,\mathbf{x}) \approx Q_X\, u_N^2(t,\mathbf{x_n}) = \sum_{j=1}^{N} \alpha_j^2(t)\beta_j(\mathbf{x}).
\tag{9}
$$

The use of the standard (6) and grouped (9) approximations in the weak form of Burgers' equation (4) leads to the GFE differential equations

$$\begin{aligned} &\mathbf{M}\,\dot{\boldsymbol{\alpha}} = -\nu\mathbf{A}\,\boldsymbol{\alpha} - \mathbf{G}(\boldsymbol{\alpha}) + \mathbf{V}(t), \\ &\boldsymbol{\alpha}(0) = \boldsymbol{\alpha_0} = \left[(u_0, \beta_i)\right]_{i=1}^{N}, \end{aligned} \tag{10}$$

where

$$\mathbf{G}(\boldsymbol{\alpha}) = \mathbf{N}\left[\mathrm{diag}(\boldsymbol{\alpha})\right]\boldsymbol{\alpha},$$

and

$$\begin{aligned} &[\mathbf{M}]_{ij} = (\beta_j,\, \beta_i), && [\mathbf{A}]_{ij} = (\beta_{j,x}, \beta_{i,x}) + (\beta_{j,y}, \beta_{i,y}), \\ &[\mathbf{N}]_{ij} = (\beta_{j,x}, \beta_i) + (\beta_{j,y}, \beta_i), && [\mathbf{V}(t)]_i = (f, \beta_i), \end{aligned} \tag{11}$$

and $(f, g) = \int_\Omega f(x)g(x)dx$ is the standard $L^2(\Omega)$ inner product. Throughout this work we use a comma to separate the index of a variable and its partial derivative. For example, in (11), $\beta_{j,x}$ denotes $\partial\beta_j/\partial x$.

The reduced computational cost of the semi-discrete GFE form (10) is due to the separation of the space and time dependent components in the nonlinear terms. As a result, the inner products, $(\beta_{j,x}, \beta_i)$ and $(\beta_{j,y}, \beta_i)$ of the nonlinear term, $\mathbf{G}(\boldsymbol{\alpha})$, may be computed *once* before integration. In contrast, a standard FE form of Burgers' equation (4) requires the re-evaluation of the nonlinear terms of the inner products at *each time step* during simulation.

The computational advantage of the GFE method over the conventional FE method for two and three dimensional Burgers' equations and viscous compressible flows is demonstrated in [13, 14]. As with the GFE method, we show that the projection of the grouped approximations onto a global POD basis also provides a computational advantage.

3. The Standard and Group POD Models for Burgers' Equation

A common practice in POD model construction is to remove the time average of the data set prior to computing the POD basis [36, 37, 38]. To this end, we write Burgers' equation (4) in terms of its fluctuation about the mean. Let the solution variable, u, be separated into the sum of its time average and fluctuation as

$$u(t, \mathbf{x}) = U(\mathbf{x}) + v(t, \mathbf{x}) \tag{12}$$

where the time average is approximated as

$$U(\mathbf{x}) = \frac{1}{S}\sum_{i=1}^{S} u(t_i, \mathbf{x}). \tag{13}$$

When the separated solution (12) is substituted into Burgers' equation (4) we obtain

$$\begin{aligned} &v_t + vv_x + vv_y - \nu(\triangle v + \triangle U) + U(U_x + U_y) + \ \ldots \\ &\qquad\qquad U(v_x + v_y) + \nu(U_x + U_y) = f, \qquad (x, y) \in \Omega, \qquad t > 0, \\ &v(t, \partial\Omega) = 0, \qquad t > 0, \\ &v(0, \mathbf{x}) = v_0, \qquad (x, y) \in \Omega. \end{aligned} \tag{14}$$

Equation (14) is the general form of the model problem considered in this work. We shall further refer to (14) as the fluctuation Burgers' equation.

3.1. The Development of the Standard POD Form of Burgers' Equation. Let the POD approximation of the fluctuation variable, $v(t,\mathbf{x})$, be written as

$$v(t,\mathbf{x}) \approx v_p(t,\mathbf{x}) = \sum_{j=1}^{M} a_j(t)\psi_j(\mathbf{x}), \tag{15}$$

where $v_p(t,\mathbf{x})$ denotes the POD approximation to the fluctuation variable, ψ_j is the jth POD mode, and $a_j(t)$ is an unknown time-dependent coefficient. The projection of the fluctuation Burgers' equation (14) onto the POD basis, $\mathbf{\Psi} = \{\psi_i\}_{i=1}^{M}$, poses the variational problem to find $v_p \in \mathbf{V}^{POD} = \text{span}\{\mathbf{\Psi}\}$ so that

$$\begin{aligned} &(v_{p,t},\psi_i) + (v_p v_{p,x} + v_p v_{p,y},\psi_i) + \ \ldots \\ &\qquad (UU_x + UU_y + U_x + U_y,\psi_i) - \nu\,(\nabla v_p,\nabla\psi_i) - \nu\,(\nabla U,\nabla\psi_i) + \ \ldots \\ &\qquad\qquad (Uv_{p,x} + Uv_{p,y} + U_x v_p + U_y v_p,\psi_i) = (f,\psi_i)\,, \qquad a_0 = (v_{p\,0},\psi_i), \end{aligned} \tag{16}$$

for $i = 1,\ldots,M$. When the POD approximation (15) is substituted into the variational problem (16), a nonlinear ODE system in terms of the unknown coefficients, $\mathbf{a} = [a_1, a_2, \ldots, a_M]^{\mathrm{T}}$, is obtained as

$$\begin{aligned} &\mathbf{M}\,\dot{\mathbf{a}} = -\mathbf{A}\,\mathbf{a} - \mathbf{N_s}(\mathbf{a}) - \mathbf{V}(t), \\ &\mathbf{a}(0) = \mathbf{a}_0 \end{aligned} \tag{17}$$

where,

$$\begin{aligned} [\mathbf{M}]_{ij} &= (\psi_j,\psi_i) \\ [\mathbf{A}]_{ij} &= (U\,\psi_{x,j} + U\,\psi_{y,j} + U_x\,\psi_j + U_y\,\psi_j,\psi_i) + \nu\,(\psi_{j,x},\psi_{i,x}) + \ \ldots \\ &\quad \nu\,(\psi_{j,y},\psi_{i,y}) \\ [\mathbf{N_s}(\mathbf{a})]_i &= \sum_{k,j=1}^{M} [(\psi_k\,\psi_{j,x},\psi_i) + (\psi_k\,\psi_{j,y},\psi_i)]\; a_k\,a_j \\ [\mathbf{V}]_i &= (-f + U\,U_x + U\,U_y,\psi_i) + \nu\,(U_x,\psi_{i,x}) + \nu\,(U_y,\psi_{i,y}) \\ [\boldsymbol{a_0}]_i &= (v_0,\psi_i)\,. \end{aligned}$$

Note that $\mathbf{M}$ is the identity matrix, since the POD modes are orthonormal. We refer to equation (17) as the standard POD form of the fluctuation Burgers' equation.

3.2. The Development of the Group POD Form of Burgers' Equation. As with the group finite element method, the group POD method requires two main steps: posing the nonlinear terms of the PDE in group form and introducing a grouped POD approximation.

The fluctuation Burgers' equation (14) may be written in grouped form as

$$\begin{aligned} &v_t + (v^2)_x + (v^2)_y - \nu(\triangle v + \triangle U) + U(U_x + U_y) + \ \ldots \\ &\qquad U(v_x + v_y) + \nu(U_x + U_y) = f, \qquad (x,y) \in \Omega, \qquad t > 0, \end{aligned} \tag{18}$$

The projection of the grouped fluctuation Burgers' equation (18) onto the POD set, $\{\psi_i\}_{i=1}^{M}$, poses the variational problem to find $v_p \in \mathbf{V}^{POD} = \text{span}\{\mathbf{\Psi}\}$ such that

$$\begin{aligned} &(v_{p,t},\psi_i) + \left((v_p^2)_x + (v_p^2)_y,\psi_i\right) + \ \ldots \\ &\qquad (UU_x + UU_y + U_x + U_y,\psi_i) - \nu\,(\nabla v_p,\nabla\psi_i) - \nu\,(\nabla U,\nabla\psi_i) + \ \ldots \\ &\qquad\qquad (Uv_{p,x} + Uv_{p,y} + U_x v_p + U_y v_p,\psi_i) = (f,\psi_i)\,, \qquad a_0 = (v_{p\,0},\psi_i), \end{aligned} \tag{19}$$

for $i = 1, \ldots, M$. Let the grouped variable, v^2, of the grouped fluctuation Burgers' equation (18) be approximated as

$$v^2(t, \mathbf{x}) \approx v_p^2(t, \mathbf{x}) = \sum_{j=1}^{M} F_j(\mathbf{a}) \psi_j(\mathbf{x}), \tag{20}$$

where each $F_j(\mathbf{a})$ is an unknown function of the POD approximation coefficients $\mathbf{a}$. When the standard POD approximation (15) and grouped POD approximation (20) are substituted into the grouped variational problem (19), the group POD form of the fluctuation Burgers' equation is obtained as

$$\begin{aligned} &\mathbf{M}\,\dot{\mathbf{a}} = -\mathbf{A}\,\mathbf{a} - \mathbf{N_g}\boldsymbol{F}(\mathbf{a}) - \mathbf{V}(t), \\ &\mathbf{a}(0) = \mathbf{a}_0 \end{aligned} \tag{21}$$

where $\mathbf{M}$ (the identity matrix) $\mathbf{A}$, $\mathbf{V}$, and $\mathbf{a_0}$ are identical to the standard POD form of the fluctuation Burgers' equation (17), $\mathbf{N_g}$ is given by

$$[\mathbf{N_g}]_{ij} \quad = \quad (\psi_{j,x}, \psi_i) \, + \, (\psi_{j,y}, \psi_i) \, ,$$

and $\boldsymbol{F}(\mathbf{a}) = [F_1, F_2, \ldots, F_M]^T$ is determined below.

To compute the nonlinear term we follow a nodal approach similar to that presented in the GFE method of Section 2.3. Let the group POD approximation (20) be evaluated with the standard POD approximation (15) at the grid nodes as

$$v^2(t, \mathbf{x}_n) \approx v_p^2(t, \mathbf{x}_n) = \sum_{j=1}^{M} F_j(\mathbf{a}) \psi_j(\mathbf{x}_n) = \left(\sum_{j=1}^{M} a_j(t) \psi_j(\mathbf{x}_n) \right)^2 . \tag{22}$$

Let $\gamma_{nj} = \psi_j(x_n)$, the value of the jth POD mode at the nth node. Then,

$$\sum_{j=1}^{M} F_j \gamma_{nj} = \left(\sum_{j=1}^{M} a_j \gamma_{nj} \right)^2 = \sum_{j,\ell=1}^{M} \gamma_{nj} \gamma_{n\ell} a_j a_\ell. \tag{23}$$

Note that $\gamma_{nj}\gamma_{n\ell} = \gamma_{n\ell}\gamma_{nj}$, that is, there is symmetry in the cross terms. Thus, for $j \neq \ell$ we may avoid computing $\gamma_{nj}\gamma_{n\ell}$ twice by writing

$$v_p^2(t, \mathbf{x_n}) = \sum_{j,\ell=1}^{M} \gamma_{nj} \gamma_{n\ell} a_j a_\ell = \hat{\boldsymbol{\gamma}}_n \, \hat{\mathbf{a}} \tag{24}$$

where $\hat{\boldsymbol{\gamma}}_n$ is a $1 \times \frac{1}{2}(M^2 + M)$ vector written as

$$\hat{\boldsymbol{\gamma}}_n = [\, \gamma_{n1}\gamma_{n1},\, 2\gamma_{n1}\gamma_{n2},\, \ldots,\, 2\gamma_{n1}\gamma_{nM},\, \gamma_{n2}\gamma_{n2},\, 2\gamma_{n2}\gamma_{n3},\, \ldots \\ 2\gamma_{n2}\gamma_{nM},\, \ldots,\, \gamma_{nM}\gamma_{nM} \,]$$

and

$$\hat{\mathbf{a}} = [a_1a_1,\, a_1a_2,\, \ldots, a_1a_M,\, a_2a_2,\, a_2a_3,\, a_2a_4,\, \ldots,\, a_2a_M,\, \ldots, a_Ma_M \,]^{\mathrm{T}}$$

is a $\frac{1}{2}(M^2 + M) \times 1$ vector. For $n = 1, 2, \ldots, N$, we may write equation (23) in matrix form as

$$\boldsymbol{\Gamma}\boldsymbol{F}(\mathbf{a}) = \hat{\boldsymbol{\Gamma}}\,\hat{\mathbf{a}}, \tag{25}$$

where $\boldsymbol{\Gamma}$ is the $N \times M$ matrix of POD mode coefficients

$$\mathbf{\Gamma} = \begin{bmatrix} \gamma_{11} & \gamma_{12} & \cdots & \gamma_{1M} \\ \vdots & \vdots & \ddots & \vdots \\ \gamma_{N1} & \gamma_{N2} & \cdots & \gamma_{NM} \end{bmatrix} \tag{26}$$

and $\hat{\mathbf{\Gamma}}$ is the $N \times \frac{1}{2}(M^2+M)$ matrix $[\hat{\boldsymbol{\gamma}}_1, \hat{\boldsymbol{\gamma}}_2, \ldots, \hat{\boldsymbol{\gamma}}_N]^{\mathrm{T}}$.

If the number of grid nodes is larger than the number of POD modes ($N > M$), in terms of $\boldsymbol{F}(\mathbf{a})$, equation (25) is overdetermined and has no solution for $\boldsymbol{F}(\mathbf{a})$. However, we do not attempt to approximate $\boldsymbol{F}(\mathbf{a})$ using (25); rather, we substitute $\hat{\mathbf{\Gamma}}\,\hat{\mathbf{a}}$ in the group POD discretization. Here, we illustrate this substitution by evaluating the nonlinear terms of the group POD form of the fluctuation Burgers' equation (21), $\mathbf{N_g}\boldsymbol{F}(\mathbf{a}) = [(\psi_{j,x}, \psi_i) + (\psi_{j,y}, \psi_i)]_{i,j=1}^{M}\, \boldsymbol{F}(\mathbf{a})$,

Assuming the POD mode takes the form of (3), when the standard POD approximation (15) is substituted into $\mathbf{N_g}$ we obtain

$$\mathbf{N_g}\boldsymbol{F}(\mathbf{a}) \approx \left\{ \sum_{j=1}^{M} \sum_{k,\ell=1}^{N} F_j \left[\gamma_{kj} \left(\int_\Omega \beta_{k,x}\beta_\ell + \beta_{k,y}\beta_\ell \, d\mathbf{x} \right) \gamma_{\ell i} \right] \right\}_{i=1}^{M}. \tag{27}$$

In matrix form, the right hand side of equation (27) becomes

$$\mathbf{N_g}\boldsymbol{F}(\mathbf{a}) \approx \mathbf{\Gamma}^T \mathbf{N}\, \mathbf{\Gamma} \boldsymbol{F}(\mathbf{a}), \tag{28}$$

where $\mathbf{\Gamma}$ and $\mathbf{N}$ are defined in equations (26) and (11), respectively. We now substitute $\hat{\mathbf{\Gamma}}\,\hat{\mathbf{a}}$ for $\mathbf{\Gamma}\boldsymbol{F}(\mathbf{a})$, from equation (25), into the right hand side of (28) to obtain

$$\mathbf{N_g}\boldsymbol{F}(\mathbf{a}) \approx \mathbf{\Gamma}^T \mathbf{N}\, \hat{\mathbf{\Gamma}}\hat{\mathbf{a}}. \tag{29}$$

Note that $\mathbf{\Gamma}^{\mathrm{T}}\mathbf{N}\hat{\mathbf{\Gamma}}$ may be computed offline. Let

$$\hat{\mathbf{N}} = \mathbf{\Gamma}^{\mathrm{T}}\mathbf{N}\hat{\mathbf{\Gamma}}, \tag{30}$$

where $\hat{\mathbf{N}}$ is $M \times \frac{1}{2}(M^2+M)$. Then, the group POD approximation may be finally written as

$$\mathbf{N_g}\boldsymbol{F}(\mathbf{a}) \approx \hat{\mathbf{N}}\,\hat{\mathbf{a}}. \tag{31}$$

With this, the GPOD model (21) becomes

$$\begin{aligned} \mathbf{M}\,\dot{\mathbf{a}} &= -\mathbf{A}\,\mathbf{a} - \hat{\mathbf{N}}\hat{\mathbf{a}} - \mathbf{V}(t), \\ \mathbf{a}(0) &= \mathbf{a_0}. \end{aligned} \tag{32}$$

This is the model used for the computations performed herein.

Note: Although we assumed the POD modes are represented as in equation (3), this is not required in general. All that must be done is to approximate $\mathbf{N_g} = \mathbf{\Gamma}^{\mathrm{T}}\mathbf{N}\mathbf{\Gamma}$, for some matrix $\mathbf{N}$. This can easily be accomplished by setting a computational grid and approximating the integrals in $\mathbf{N_g}$ with quadrature.

4. The Computational Cost of Group and Standard Nonlinear Terms

In this section we present a general implementation of the group and standard POD models for the fluctuation Burgers' equation and compare the number of multiplication operations required to compute their nonlinear terms. The group POD form of the nonlinear term of the fluctuation Burgers' equation will be shown to require $M^3 - \frac{1}{2}M^2 - \frac{1}{2}M$ less floating point operations (flops) than the standard POD

implementation, where one flop is taken as an addition, subtraction, multiplication or division floating point operation, and M is the model order.

Throughout, we assume the nonlinear terms in the group POD model are computed using equation (31), as described in the previous section.

4.1. The Cost of the Standard POD Implementation. Recall the standard POD form of the fluctuation Burgers' equation (17). When the POD mode (3) is substituted into (17) we obtain

$$\begin{aligned} \mathbf{M}\,\dot{\mathbf{a}} &= -\mathbf{A}\,\mathbf{a} - \mathbf{N_s}(\mathbf{a}) - \mathbf{V}(t), \\ \boldsymbol{a}(0) &= \boldsymbol{a_0}, \end{aligned}$$

where

$$\begin{aligned} \mathbf{M} &= \mathbf{\Gamma}^{\mathrm{T}}\,\mathbf{M}_1\,\mathbf{\Gamma}, \\ \mathbf{A} &= \mathbf{\Gamma}^{\mathrm{T}}\,[\,\mathbf{A}_1 + \nu\,\mathbf{A}_2 + \mathbf{A}_3]\,\mathbf{\Gamma}, \\ \mathbf{N_s}(\mathbf{a}) &= \mathbf{a}^{\mathrm{T}}\,\mathbf{\Gamma}^{\mathrm{T}}\,\mathbf{E}\,\mathbf{\Gamma}\,\mathbf{a}, \\ \mathbf{V} &= \mathbf{\Gamma}^{T}\,[\,\nu\,\mathbf{V}_1 + \mathbf{V}_2 - \mathbf{V}_3\,], \\ \boldsymbol{a_0} &= \mathbf{\Gamma}^{T}\,\mathbf{T}, \end{aligned}$$

and

$$\begin{aligned} &[\mathbf{M}_1]_{ij} = (\beta_j, \beta_i), && [\mathbf{A}_1]_{ij} = (U\beta_{x,j}, \beta_i) + (U\beta_{y,j}, \beta_i), \\ &[\mathbf{A}_2]_{ij} = (\beta_{j,x}, \beta_{i,x}) + (\beta_{j,y}, \beta_{i,y}), && [\mathbf{A}_3]_{ij} = (U_x\beta_j, \beta_i) + (U_y\beta_j, \beta_i), \\ &[\mathbf{E}]_{ijk} = (\beta_{j,x}\,\beta_k, \psi_i) + (\beta_{j,y}\,\beta_k, \psi_i), && [\mathbf{V}_1]_i = (U_x, \beta_{i,x}) + (U_y, \beta_{i,y}), \\ &[\mathbf{V}_2]_i = (UU_x, \beta_i) + (UU_y, \beta_i), && [\mathbf{V}_3]_i = (f, \beta_i), \\ &[\mathbf{T}]_i = (v_0, \beta_i), \end{aligned}$$

for $i, j = 1, \ldots, N$ and $k = 1, \ldots, M$. The above ODE system (33) is the computational form of the standard POD model of Burgers' equation implemented in this work. The nonlinear term, $\mathbf{N_s}(\mathbf{a})$, may be written as

$$\begin{bmatrix} a_k\,\gamma_{\ell k}\;(\beta_\ell\,\beta_{p,x} + \beta_\ell\,\beta_{p,x}, \psi_1)\;\gamma_{pj}\,a_j \\ a_k\,\gamma_{\ell k}\;(\beta_\ell\,\beta_{p,x} + \beta_\ell\,\beta_{p,x}, \psi_2)\;\gamma_{pj}\,a_j \\ \vdots \\ a_k\,\gamma_{\ell k}\;(\beta_\ell\,\beta_{p,x} + \beta_\ell\,\beta_{p,x}, \psi_M)\;\gamma_{pj}\,a_j \end{bmatrix} = \begin{bmatrix} \mathbf{a}^T\,\mathbf{S}_1\,\mathbf{a} \\ \mathbf{a}^T\,\mathbf{S}_2\,\mathbf{a} \\ \vdots \\ \mathbf{a}^T\,\mathbf{S}_M\,\mathbf{a} \end{bmatrix} \tag{33}$$

where $\mathbf{a}$ is an $M \times 1$ vector and $\mathbf{S}_i = \mathbf{\Gamma}^T\,\mathbf{E}_i\,\mathbf{\Gamma}$ is a dense, nonsymmetric, $M \times M$ matrix. To our knowledge, the right hand side of equation (33) has no more computationally efficient form and is written as implemented in our code.

The computation of each of the M rows of (33) requires $2M^2 + M - 1$ flops. Thus, the total number of flops required to compute the nonlinear terms for the standard POD implementation is as follows:

$$\text{Cost of standard nonlinear terms} = 2M^3 + M^2 - M. \tag{34}$$

4.2. The Cost of the Group POD Implementation. Recall the group POD form of the fluctuation Burgers' equation (29). When the POD mode (3) is substituted into (29) we obtain

$$\begin{aligned} \mathbf{M}\,\dot{\mathbf{a}} &= -\mathbf{A}\,\mathbf{a} - \hat{\mathbf{N}}\hat{\mathbf{a}} - \mathbf{V}(t), \\ \mathbf{a}(0) &= \mathbf{a_0}, \end{aligned} \tag{32}$$

where $\mathbf{M}$, $\mathbf{A}$, $\mathbf{V}(t)$, and $\mathbf{a}_0$ are identical to the standard implementation (33), and $\hat{\mathbf{N}} = \mathbf{\Gamma}^{\mathrm{T}}\mathbf{N}\hat{\mathbf{\Gamma}}$, equation (30) of Section 3.2. Equation (32) is the form of the group POD model for the fluctuation Burgers' equation implemented in this work.

In Section 3.2, we showed that $\hat{\mathbf{N}}$ is size $M \times \frac{1}{2}(M^2 + M)$ and $\hat{\mathbf{a}}$ is size $\frac{1}{2}(M^2 + M) \times 1$. The product $\hat{\mathbf{N}}\,\hat{\mathbf{a}}$ requires $M^3 + M^2 - M$ flops, plus $\frac{1}{2}(M^2 + M)$ flops to compute $\hat{\mathbf{a}}$. Thus, the total number of operations to compute the nonlinear group POD term is

$$\text{Cost for group nonlinear term} = M^3 + \frac{3}{2}M^2 - \frac{1}{2}M. \tag{35}$$

By comparison, the computation of the nonlinear term of the group POD model requires $M^3 - \frac{1}{2}M^2 - \frac{1}{2}M$ flops less than the standard POD implementation.

We further investigate the computational cost of the group POD method in Section 5, where a comparison of total integration times of the group and standard POD models for the fluctuation Burgers' equation is performed.

5. Numerical Results

In this section, we assess the accuracy and computational cost of the group POD model of the fluctuation Burgers' equation (32) with a comparison to the standard POD implementation (33). Simulations show that the group POD model is as accurate and more efficient than the standard POD model for the fluctuation Burgers' equation.

5.1. The Accuracy of the Group POD Method. To quantify the accuracy of each model, an analytical benchmark solution for Burgers' equation was created using the method of manufactured solutions (MMS). The MMS is a verification procedure for computer codes that solve partial differential equations (PDEs). In the MMS, an analytical benchmark solution is manufactured by substituting an analytical function into each term of a PDE and appending the result as an analytical forcing on the system. The manufactured solution chosen for this analysis was

$$u(t, \mathbf{x}) = 10xy(x-1)(y-1)[\sin(2xt)e^{-\frac{t}{2}} + \cos(yt)e^{-\frac{t}{4}} + \sin(xyt)e^{-t}]. \tag{36}$$

This function (36) was chosen, in part, to satisfy the zero boundary conditions and ensure the influence of the nonlinear terms during the simulation. More information on the guidelines of choosing a manufactured solution may be found in [15, 17, 19]. We computed the analytical forcing function, f, by substituting the manufactured solution into each term in the left hand side of Burgers' equation (4), using MATLAB's symbolic toolbox to perform the calculation.

A POD basis was computed with the method of snapshots over the time interval $[0, 10]$ seconds. For these computations, the exact solution (36) was projected onto a piecewise linear basis on a uniform triangular grid on $[0, 1] \times [0, 1]$. The grid resolution and time step size of the snapshot set was determined based on the convergence of the POD eigenvalues and POD modes. To this end, we selected a

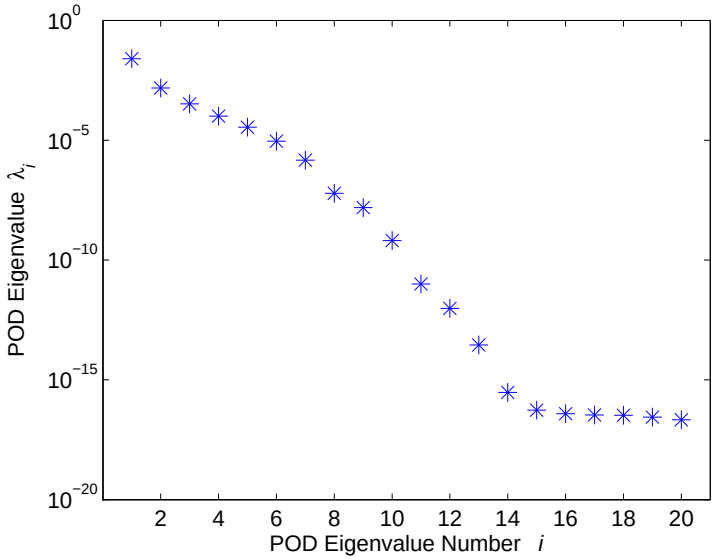

FIGURE 1. POD eigenvalues 1 to 20 computed from a 1025 snapshot 65×65 node snapshot set of the benchmark solution (36)

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65×65 node grid with 1025 snapshots, which was sufficient for convergence. Figure 1 is a semi-log plot of the POD eigenvalues of the converged POD basis.

Standard and group POD models of the fluctuation Burgers' equation were constructed for POD basis sizes ranging from 1 to 15 modes. Each reduced model was integrated over the time interval $0 \leq t \leq 10$ seconds with Matlab's `ode15s` solver, having absolute and relative error tolerances of of 10^{-5} and 10^{-3}, respectively (the default settings). For each integration, the initial condition was computed from (36) as $u(0, \mathbf{x}) = 10xy(x-1)(y-1)$. The parameter ν was specified as $1/100$.

To quantify the accuracy of the group and standard POD models, a relative global error between the simulations and the benchmark solution (36) was evaluated as

$$\text{err}_r = \frac{\|u(t_i) - u^r(t_i)\|_{L^2}}{\|u(t_i)\|_{L^2}}, \tag{37}$$

where $\|\cdot\|_{L^2}$ is the L^2 norm evaluated as $\|\cdot\|_{L^2} = \left(\int_\Omega |\cdot|^2 d\mathbf{x}\right)^{1/2}$, t_i denotes the ith point in time, and r denotes the order of the corresponding POD model.

Figures 2 and 3 are plots of the relative global error, err_r, versus model order, r, at various points in time during the simulation of the group POD model and standard POD model of Burgers' equation, respectively. For the points in time shown, the relative global error of each model is shown to approximately converge to values on the order of 10^{-4} to 10^{-3} with increasing POD basis size. Thus, we find the group POD model of the fluctuation Burgers' equation (33) as accurate as the standard POD model for the fluctuation Burgers' problem (32).

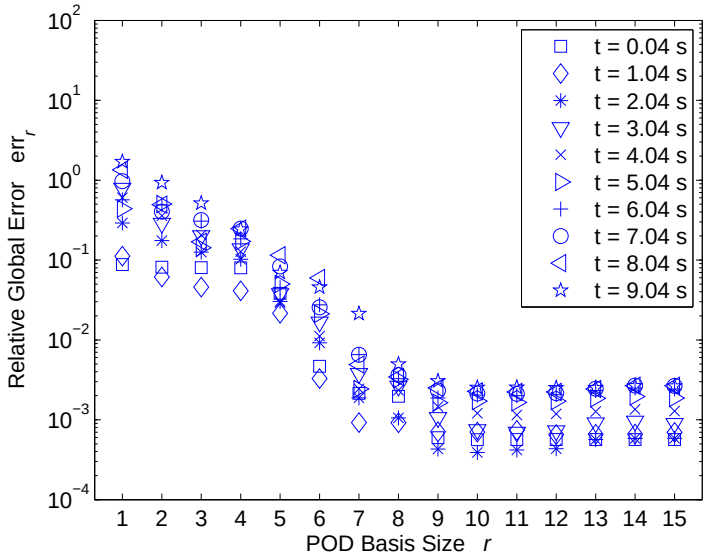

FIGURE 2. Semilog plot of relative global error versus POD basis size at various points in time for the simulation of the group POD model of the fluctuation Burgers' equation

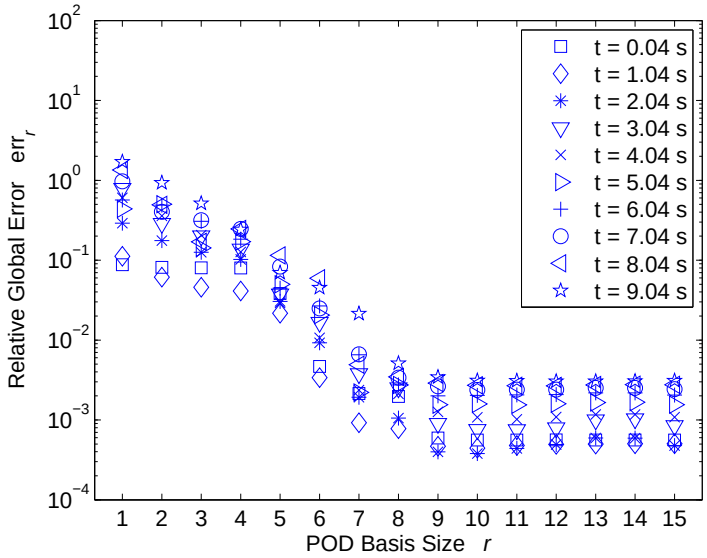

FIGURE 3. Semilog plot of relative global error versus POD basis size at various points in time for the simulation of the standard POD model of the fluctuation Burgers' equation

5.2. The Efficiency of the Group POD Method. In this section, we further investigate the computational cost of the group POD model (32) by comparing total integration time to the standard POD implementation (33).

In the previous section, we used an analytical forcing to construct a benchmark solution to quantify model accuracy. However, the discretization of the cumbersome analytical forcing function was required at each time step, which caused the integration times of each model to be dominated by the discretization of the forcing, f. To clearly assess the cost of computing the nonlinear terms of each model we solve an unforced fluctuation Burgers' equation ($f = 0$).

The unforced form of the Burgers' problem, presented in Section 2.3, was solved using the group finite element (GFE) method. We chose the initial condition to be defined by the function

$$u_0 = \sin(y\frac{\pi}{2})\,\sin(x\frac{\pi}{2}) \tag{38}$$

for $(x, y) \in [\frac{1}{10}, \frac{3}{10}] \times [\frac{1}{10}, \frac{3}{10}]$ and 0 elsewhere. Figure 4 is surface plot of the initial condition (38) used in the GFE simulation of Burgers' equation The GFE form of

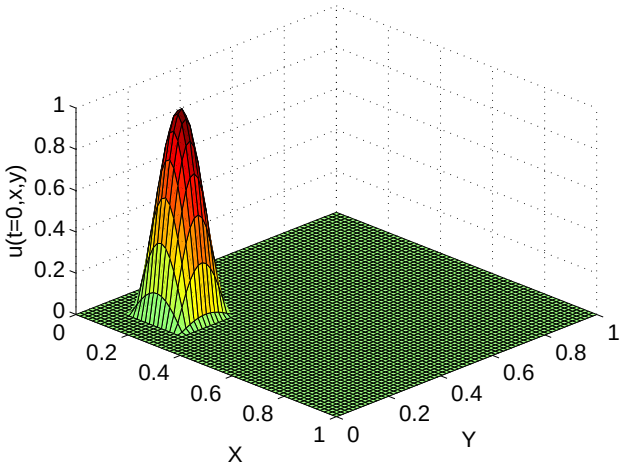

FIGURE 4. Surface plot of initial condition (38) used in the GFE simulation of Burgers' equation

Burgers' equation (10) was solved over the time interval $0 \le t \le 5$ seconds with Matlab's `ode15s` solver using the default settings. The parameter ν was specified as 1/100.

The POD basis used to construct subsequent POD models was computed with a snapshot set of the GFE simulation on a uniform triangular grid on $[0, 1] \times [0, 1]$ over the time interval $0 \le t \le 5$ seconds. The spatial and temporal refinement of the snapshot set was determined based on the convergence of the POD eigenvalues and POD modes. To this end, we selected a 33×33 node grid with 1025 snapshots, which was sufficient for convergence. Figure 5 is a plot of the POD eigenvalues computed from the converged POD basis.

Standard and group POD models of the fluctuation Burgers' equation were constructed for POD basis sizes ranging from 1 to 25 modes. Each reduced model was integrated over the time interval $0 \le t \le 5$ seconds using a fourth order Runge-Kutta (RK4) solver having a constant time step size of 1/1000 seconds. The RK4

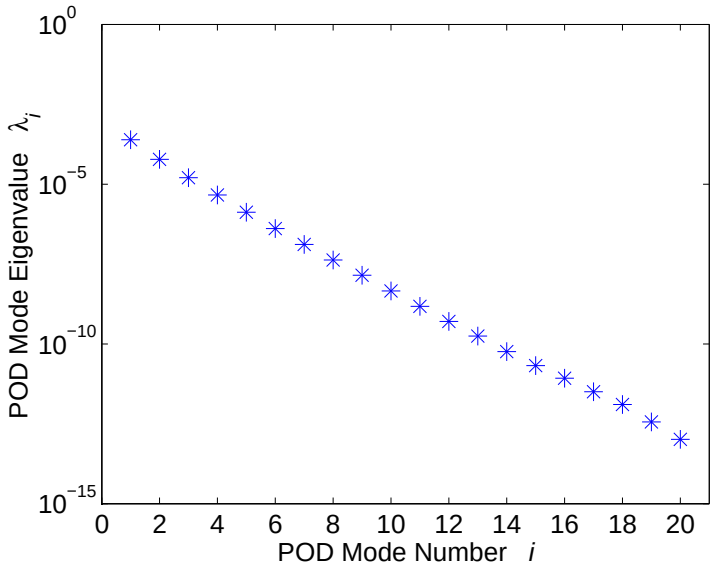

FIGURE 5. POD eigenvalues 1 to 20 computed from a 33×33 node 1025 snapshot snapshot set of the unforced GFE simulation of Burgers' equation (10)

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solver was chosen because the simplicity of its implementation allowed a clear assessment of the link between total integration time and the cost of computing the nonlinear terms of the Burgers' POD models.

To quantify the total elapsed time for each integration, Matlab's tic-toc feature was used. The tic-toc command records real time between two points in a code, specified by tic and toc. We applied tic-toc immediately before and after the RK4 solver for all simulations.

Group and standard POD models of orders 1 through 25 were integrated 100 times and the average integration time for each model order and type was computed. Figure 6 is a plot of the average total integration time versus model order of the standard (33) and group (32) POD implementations. The standard deviation of the 100 simulation times for each model was on the order of 10^{-2} seconds. From Figure 6, the group POD implementation (33) is shown to provide an increasing savings with model order over the standard POD implementation (32), which is consistent with the operation count savings, $r^3 - \frac{1}{2}r^2 - \frac{1}{2}r$, presented in Section 4.2.

6. Extension to Other Nonlinear Problems

In this work, we applied the group POD method to the quadratic nonlinearity of Burgers' equation as model problem for an incompressible form of the Navier-Stokes equations. We may also apply the group POD method to any equation with a polynomial nonlinearity, for example, the compressible Navier-Stokes equations. In foresight of this potential application, we provide a general extension of the group POD method to a cubic nonlinearity.

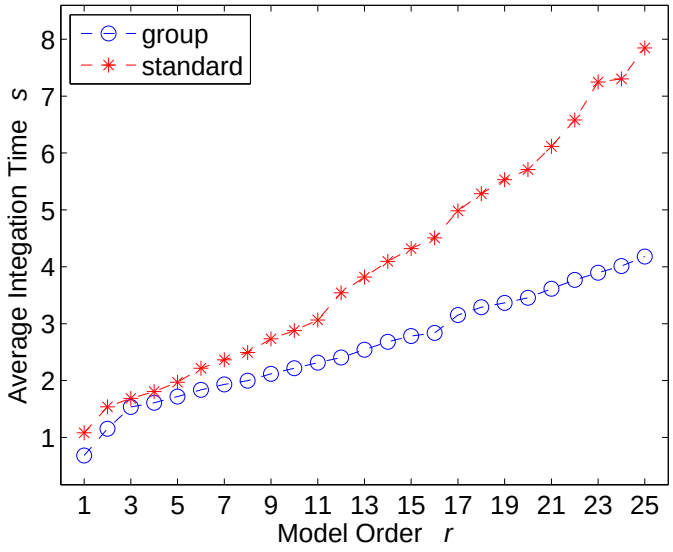

FIGURE 6. Total integration time (averaged over 100 trials) of standard and group POD models of Burgers equation versus model order

Consider a grouped cubic term $v^3(t,\mathbf{x})$. Following the approach in Section 3.2, let the cubic term be approximated as

$$v_p^3(t,\mathbf{x}) = \sum_{k=1}^{M} F_k(\mathbf{a})\psi_k(\mathbf{x}) \tag{39}$$

where $F_k(\mathbf{a})$ is an unknown function of the group POD coefficient. Let us evaluate $v^3(t,\mathbf{x})$ at the nodes using the standard POD approximation as

$$v_p^3(t,\mathbf{x}_n) = \sum_{k=1}^{M} F_k(\mathbf{a})\psi_k(\mathbf{x}_n) = \left(\sum_{j=1}^{M} a_j\gamma_{nj}\right)^3 = \sum_{k,l,m=1}^{M} \gamma_{nk}\gamma_{nl}\gamma_{nm}a_k a_l a_m. \tag{40}$$

As with the quadratic nonlinearity of Section 3.2, Equation (40) may be written in similar matrix form as

$$\mathbf{\Gamma}\boldsymbol{F}(\mathbf{a}) = \hat{\mathbf{\Gamma}}\,\hat{\mathbf{a}}, \tag{41}$$

where $\hat{\mathbf{\Gamma}}$ and $\hat{\boldsymbol{a}}$ are constructed in a pattern similar to the quadratic terms presented in Section 3.2. This pattern may be observed by expanding the third term of equation (40) for $M = 2, 3$, and 4. By taking advantage of the symmetry in the cross terms ($\gamma_{nk}\gamma_{nl}\gamma_{nj} = \gamma_{nl}\gamma_{nj}\gamma_{nk} = \gamma_{nj}\gamma_{nk}\gamma_{nl}$), in terms of operation counts, an even larger computational savings is obtained over the standard POD implementation. We expect these savings to be realized in simulations of cubic group POD models.

7. Conclusions

In this work, we submitted the group proper orthogonal decomposition (POD) method to write nonlinear POD based reduced order models with an improved

computational cost in the nonlinear terms. The group POD method was developed by extending ideas from group finite elements to global POD basis functions.

Here, a scalar, two-dimensional Burgers' equation was used as a model problem. The accuracy of the group POD model of Burgers' equation was shown to be similar to the standard POD model. The group POD method was also shown to provide a reduced computational cost over the standard POD implementation with flop counts and experiments quantifying total integration times. A brief extension of the group POD method to cubic nonlinearities was also provided. On the basis of comparable accuracy and improved economy, the group POD method seems to be a promising technique for nonlinear model reduction.

Future work includes testing the group POD method on incompressible and compressible forms of the Navier-Stokes equations. A complete convergence analysis of the method (as in [7, 8, 9, 29]) would also be of interest.

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