Lagrangian basis method for dimensionality reduction of convection dominated nonlinear flows

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Foundations of a new projection-based model reduction approach for convection dominated nonlinear fluid flows are summarized. In this method the evolution of the flow is approximated in the Lagrangian frame of reference. Global basis functions are used to approximate both the state and the position of the Lagrangian computational domain. It is demonstrated that in this framework, certain wave-like solutions exhibit low-rank structure and thus, can be efficiently compressed using relatively few global basis. The proposed approach is successfully demonstrated for the reduction of several simple but representative problems.

Key words:

1. Introduction

Numerical simulation of nonlinear fluid flows often requires prohibitively large computational resources. High-fidelity simulations of high-Reynolds numbers flows, high-speed compressible flows, and combustion often require very fine spatial and temporal discretizations to accurately resolve the multi-scale dynamics. There are significant scientific and engineering benefits to developing model reduction techniques that are capable of delivering physics-based, low-dimensional models.

Most existing model order reduction (MOR) approaches are based on projection (Benner et al. 2015). In projection-based MOR, the states of the flow are approximated in a low-dimensional subspace and Galerkin or Petrov-Galerkin projection is used to yield reduced-order models capable of, in principle, delivering new solutions at a fraction of the computational costs of the original high-fidelity model (HFM).

Despite the efficacy and success of MOR approaches, wave-like solutions, or solutions featuring moving sharp gradients, shocks or interfaces remain a major hurdle for projection-based MOR. It is well known that this hurdle is the result of the spectral decomposition of the solution, and not the type of basis used. It is simply not possible to efficiently compress solutions with moving discontinuities or sharp gradients using a summation of products of global spatial and temporal basis functions. Over the years, several remedies have been proposed. For example, local basis (Amsallem et al. 2012), domain decomposition (Lucia 2001) or basis splitting (Carlberg 2015) algorithm have been developed. Unfortunately, the complexity of these algorithms often make extensions

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to higher dimensions not straight forward. Moreover, there are many applications where remaining in the global basis ansatz is desired; for example, global basis generated via proper orthogonal decomposition (POD) correspond to coherent structures in a turbulent flow (Lumley 1970). Other attempts have focused on exploiting symmetry, self similarity, and coordinate transformations (Rowley & Marsden 2000; Rowley et al. 2003; Kavousanakis et al. 2007; Rapun & Vega 2010; Gerbeau & Lombardi 2014) but these methods are usually limited to specific dynamical systems and to problems dominated by a single wave direction.

The main contribution of the present work is the development of a simple and general method for low-dimensional modeling of a large class of solutions characterized by travelling wave, moving shocks, sharp gradients and discontinuities. In this method, the reduction is performed in the Lagrangian frame of reference. That is, global basis functions are used to approximate both the state and the locations of the temporally evolving Lagrangian computational grid. It is demonstrated that in this framework, certain wave-like solutions exhibit low-rank structure and thus, can be efficiently compressed using relatively few global basis.

The paper is organized as follows. In §2, the traditional Eulerian MOR approach recapitulated. In §3, the new proposed Lagrangian MOR is laid out and in §4, several simple yet representative problems are considered. Finally, in §5, the main results are summarized and future prospects are laid out.

2. Traditional Eulerian projection-based model order reduction

We recapitulate the traditional Eulerian projection-based MOR approach as a starting point for our innovation in §3. Consider the following scalar, one-dimensional convection-diffusion equation

$$\frac{\partial w(x,t)}{\partial t} + f_1(x,t,w) \frac{\partial w(x,t)}{\partial x} = f_2(x,t,w) \frac{\partial^2 w(x,t)}{\partial x^2}, \quad (2.1)$$

in the domain \((x,t) \in [x_a, x_b] \times [0, T]\), equipped with initial conditions \(w(x,0) = w_0(x)\), and appropriate boundary conditions at \(x_a\), and \(x_b\). It is assumed throughout the reminder of this paper that (2.1) is discretized uniformly in space \(x = (x_1, \ldots, x_N)^T\) using standard techniques such as finite-volume or finite-elements. For the sake of simplicity, and without any loss of generality, time discretization is performed using the first-order implicit Euler scheme. Hence, if \(t^0 = 0 < t^1 < \cdots < t^{N_t} = T\) denotes a discretization of the time interval \([0, T]\) and \(w(x,t^n) \approx w^n = (w_1^n, \ldots, w_N^n)^T \in \mathbb{R}^N\), for \(n \in \{1, \ldots, N_t\}\), the discrete counterpart of (2.1) at time-step \(n\) is

$$R(w^n) = w^n - w^{n-1} + \Delta t f_1^n(w^n) \odot (D_1 w^n) - \Delta t f_2^n(w^n) \odot (D_2 w^n) = 0, \quad (2.2)$$

where \(\odot\) denotes the Hadamard product, \(D_1 \in \mathbb{R}^{N \times N}\), and \(D_2 \in \mathbb{R}^{N \times N}\) are the discrete approximations of the first and second spatial derivatives, respectively.

In traditional projection-based MOR, the solution is approximated by a global trial subspace

$$w^n \approx \tilde{w}^n = w_0 + Ua^n, \quad (2.3)$$

where the columns of \(U \in \mathbb{R}^{N \times k}\) contain the basis for this subspace, and \(a^n \in \mathbb{R}^k\) denotes the generalized coordinates of the vectors in these basis. Substituting (2.3) into (2.2) and projecting onto test basis \(\Phi \in \mathbb{R}^{N \times k}\), yields the square system

$$\Phi^T R(w_0 + Ua^n) = 0, \quad (2.4)$$

where \(\Phi = U\) in the case of a Galerkin projection.
For the sake of brevity, we confine our attention to basis generated via the proper orthogonal decomposition (POD) (Sirovich 1987; Holmes et al. 2012; Noack et al. 2011). It is emphasized however that the proposed approach is applicable to any basis generation method; such as, for example, the dynamic mode decomposition (DMD) and Koopman modes (Rowley et al. 2009; Schmid 2010; Chen et al. 2012; Williams et al. 2015; Wynn et al. 2013; Kutz et al. 2016; Proctor et al. 2016; Brunton et al. 2015). In POD, we seek a low-rank approximation to the snapshot matrix:

$$\min_{\text{rank}(\tilde{X})=k} \| X - \tilde{X} \|_F, \quad (2.5)$$

where the snapshot matrix $X \in \mathbb{R}^{N \times K}$ contains the solution of the HFM given by (2.2). In other words, $[X]_{:,i} = w^i$ for $i = 1, \ldots, K$. Here, Matlab row-column subscript notation is used. For example, $[A]_{a:b,;}$ identifies a matrix formed by extracting rows $a$ to $b$, and all columns from the matrix $A$. The main focus of the proposed work is on dynamic problems and on snapshots associated with different time instances for one set of parameters. However, in general, the snapshot matrix can contain solutions for any combination of parameters, that is, for some specific time $t$, some specific set of flow parameters and/or some boundary or initial conditions underlying the governing equations.

The rank constraint is taken care of by representing the unknown matrix as $\tilde{X} = UV$ where $U \in \mathbb{R}^{N \times k}$ and $V \in \mathbb{R}^{k \times K}$, so the problem becomes

$$\min_{U,V} \| X - UV \|_F. \quad (2.6)$$

The solution of the above low-rank approximation problem is given by the Eckart-Young-Mirsky theorem (Eckart & Young 1936; Mirsky 1960) via the singular value decomposition (SVD) of $X$. Specifically, $X = UV$, where $U = [U^*]_{:,1:k}$ and $V = [\Sigma V^*T]_{1:k,;}$ where $X = U^* \Sigma V^* T$.

3. Lagrangian projection-based model order reduction

In this section, the proposed new Lagrangian dimensionality reduction approach is laid out. Technical details are outlined in §3.1 and §3.2 while several algorithms for computing the optimal Lagrangian basis are presented in §3.3. Finally, in §3.4, we discuss the issues and remedies for Lagrangian grid entanglement.

3.1. Lagrangian formulation of high-fidelity model

For the purpose of the proposed dimensionality reduction approach, the governing equations (2.1) are formulated in the Lagrangian frame of reference

$$\frac{dx}{dt} = f_1(x, t, w), \quad (3.1a)$$
$$\frac{\partial w}{\partial t} = f_2(x, t, w) \frac{\partial^2 w}{\partial x^2}. \quad (3.1b)$$

The discrete counterpart of (3.1) at time-step $n$ is

$$R_x(x^n) = x^n - x^{n-1} - \Delta t f_1^n(w^n) = 0, \quad (3.2a)$$
$$R_w(w^n) = w^n - w^{n-1} - \Delta t f_2^n(w^n) \odot (D_x^2 w^n) = 0, \quad (3.2b)$$
where $x^n = (x^n_1, \ldots, x^n_N)^T$ denotes the locations of the Lagrangian computational grid at time level $n$, and $D^n_2$ denotes the discrete approximation of the second derivative on the Lagrangian grid at time level $n$.

### 3.2. Nonlinear model reduction

In the proposed new dimensionality reduction approach, the Lagrangian solution is approximated by a global trial subspace

$$
x^n \approx \tilde{x}^n = x_0 + U_x a^n_x, \quad (3.3a)
$$

$$
w^n \approx \tilde{w}^n = w_0 + U_w a^n_w, \quad (3.3b)
$$

where the columns of $U_x \in \mathbb{R}^{N \times k}$ and $U_w \in \mathbb{R}^{N \times k}$ contain the basis for the corresponding subspace, and $a^n_x \in \mathbb{R}^k$ and $a^n_w \in \mathbb{R}^k$ denote the generalized coordinates of the vectors in these basis. Substituting $\tilde{x}^n$ into (3.2) and projecting onto test basis $\Phi_x \in \mathbb{R}^{N \times k}$ and $\Phi_w \in \mathbb{R}^{N \times k}$; yields the square system

$$
\Phi_x^T R_x (x_0 + U_x a^n_x) = 0, \quad (3.4a)
$$

$$
\Phi_w^T R_w (w_0 + U_w a^n_w) = 0, \quad (3.4b)
$$

where $\Phi_x = U_x$ and $\Phi_w = U_w$ in the case of a Galerkin projection.

### 3.3. Construction of optimal Lagrangian global basis functions

For cases where the HFM is formulated in the Lagrangian frame of reference, that is, when the governing equations are in the form of (3.2), construction of Lagrangian basis follows a procedure very similar to traditional POD. Specifically, we solve the low-rank approximation problem given by (2.6), for a snapshot matrix $X \in \mathbb{R}^{N \times k}$ containing solution snapshots computed by (3.2). In other words, $[X]_{:,i} = \begin{bmatrix} x^i & w^i \end{bmatrix}$ for $i = 1, \ldots, K$. Therefore, the optimal Lagrangian basis corresponds to $U_x = [U]_{1:N,1:k}$ and $U_w = [U]_{N+1:2N,1:k}$, where $U$ are the left singular vectors of the snapshot matrix $X$.

For cases where the HFM is formulated in the Eulerian frame of reference, that is, when the governing equations are in the form of (2.1), Lagrangian basis cannot be constructed by solving the standard low-rank approximation problem because Eulerian HFM typically do not provide the grid deformation $x^i$. Thus, it is not possible to form the snapshot matrix $[X]_{:,i} = \begin{bmatrix} x^i & w^i \end{bmatrix}$. For these cases, it is proposed here to construct Lagrangian basis by solving a modified low-rank approximation problem

$$
U_x, V_x, U_w, V_w \min \| X - \mathcal{P}_{U_x, V_x} (U_w, V_w) \| F, \quad (3.5)
$$

where $\mathcal{P}_{U_x, V_x}$ is the interpolation from the Lagrangian grid $x^i = U_x [V_x]_{:,i}$ to the Eulerian grid $x$, and the snapshot matrix $X \in \mathbb{R}^{N \times K}$ contains the Eulerian snapshots on the stationary Eulerian computational grid, $x$. Unlike problem (2.6), problem (3.5) does not have a closed form solution. Consequently, it must be solved using an iterative method. In this work, (2.6) is solving in Matlab using the lsqnonlin unconstrained optimization algorithm. Forward finite differences are used to approximate the gradients and the linear interp1 algorithm is used for the interpolation, $\mathcal{P}_{U_x, V_x}$.

### 3.4. Lagrangian grid entanglement

In the proposed Lagrangian MOR approach, the evolution of the Lagrangian spatial grid is approximated in a low-dimensional subspace, $x^i \approx U_x a^i_x$. Unfortunately, this
low-dimensional approximation is not guaranteed to preserve the topological properties of the original HFM simulation. Indeed, for some particular cases, the low-dimensional Lagrangian grid becomes severely distorted leading to numerical instabilities. For these cases, particularly those featuring strong shocks, we propose the following modification to the model reduction procedure. Instead of solving the diffusion step in the Lagrangian frame, as in (3.4b), the state basis $U_w$ are interpolated from the Lagrangian to the stationary Eulerian grid at every time level $n$ and the projection is performed in the Eulerian frame. Therefore, (3.4b), is replaced with the following

$$
\hat{\Phi}_T^T \hat{R}_w (\hat{w}_0 + \hat{U}_w a^n_w) = 0,
$$

where $\hat{\Phi}_w = \mathcal{P}_x \Phi_{xa} (U_w)$, $\hat{U}_w = \mathcal{P}_x \Phi_{xa} (U_w)$, and $\hat{w}_0 = \mathcal{P}_x \Phi_{xa} (w_0)$, are the interpolated basis and initial conditions and $\hat{R}_w$ is the diffusion step in the Eulerian frame, defined as

$$
\hat{R} (w^n) = w^n - w^{n-1} - \Delta t f_2^n (w^n) \odot (D_2 w^n) = 0.
$$

4. Applications

In this section, the proposed approach is applied to several canonical one-dimensional problems. In §4.1 and 4.2 results for the reduction of the convection-diffusion and Burger’s equation are presented. While in §4.3 results for the steady, quasi-1D Euler equation parametrized by the throat diameter of a converging-diverging nozzle are summarized.

4.1. Convection-diffusion equation

The proposed approach is first applied to the reduction of the scalar linear convection equation and a high Péclet number convection-diffusion equation. Specifically, we consider \([2.1]\) with $f_1(x,t,w) = 1$, $f_2(x,t,w) = 1/Pe$, $w(x,0) = 0.5 e^{-(x-0.3)^2/0.05^2}$, $w(0,t) = 0$, for $(x,t) \in [0,1.5] \times [0,1]$, where $Pe = \infty$ and $Pe = 10^3$.

Two HFMs are constructed for this case; one in the Eulerian frame, as in (2.2), and one in the fully Lagrangian frame, as in (3.2). For both models, a second-order central finite difference discretization is used. $N = 2000$ grid points are used to discretized the domain $0 \leq x \leq 1.5$. A total of $K = 2000$ Eulerian and Lagrangian snapshots are collected. Eulerian and Lagrangian basis are constructed by solving (2.6). Eulerian ROMs are solved in the form of (2.4) and Lagrangian ROMs are solved in the fully Lagrangian frame, as in Eq.(3.4a) and Eq.(3.4b). Galerkin projection is used in all cases so $\Phi = U$ and $\Phi_x = U_x$, $\Phi_w = U_w$.

ROM solutions for the convection equation and the high Péclet number convection-diffusion equation are illustrated in Fig. 1 and Fig. 2 respectively. In both cases, traditional Eulerian ROMs and the new, Lagrangian ROMs, are illustrated in in the (a) and (b) subfigures. Solutions are plotted for $t = 0, 1/3, 2/3, 1$.

In both figures, thick grey lines correspond to the HFM models, while the dashed green and solid red lines correspond to $k = 2$, and $k = 5$ ROMs, respectively.

Convergence of Eulerian and Lagrangian ROMs of the high Péclet number convection-diffusion are illustrated in Fig. 4a, where error is defined as Frobenius distance between HFM and its ROM. For both cases considered, lagrangian ROMs significantly outperform the Eulerian ROMs in all cases considered.
4.2. Burger’s equation

The proposed approach is next applied to the reduction of a convection-dominated Burger’s equation. Specifically, we consider (2.1) with \( f_1(x, t, w) = w(x, t), \) \( f_2(x, t, w) = 1/Re, \) \( w(x, 0) = 0.8 + 0.5 \, e^{-(x-0.3)^2/0.1^2}, \) \( w(0, t) = 0, \) for \( (x, t) \in [0, 1.5] \times [0, 1], \) where \( Re = 10^3. \) As before, two HFM are constructed, one in the Eulerian frame, as in (2.2), and one in the fully Lagrangian frame, as in (3.2). For both models, a second-order central finite difference discretization is used. \( N = 2000 \) grid points are used to discretized the domain \( 0 \leq x \leq 1.5. \) Total of \( K = 2000 \) Eulerian and Lagrangian snapshots are collected. Eulerian and Lagrangian basis are constructed by solving (2.6). Eulerian ROMs are solved in the form of (2.4). Due to the significant Lagrangian grid entanglement caused by the nonlinear convection term in the Burger’s equation, the Lagrangian ROMs are solved using the modified diffusion step; i.e. Eq. (3.4b) is replaced with (3.6). Galerkin projection is used in both cases.

Solutions at \( t = 0, 1/3, 2/3, 1 \) derived using the traditional and the new proposed approach are illustrated in Fig. 3a and Fig. 3b respectively. Convergence of the Eulerian and Lagrangian ROMs are illustrated in Fig. 4b. The Lagrangian ROMs significantly outperform the Eulerian ROMs. For example, a \( k = 1 \) Lagrangian ROM has approximately the same error as a \( k = 20 \) Eulerian ROM. Note that Lagrangian ROMs only up to \( k = 5 \) are considered. After \( k = 5, \) some of the interpolated
Lagrangian basis $\hat{U}_w$ become linearly dependent and thus, no further performance gain can be expected.

4.3. Quasi-1D Euler equation

Finally, the proposed approach is applied to the parametric, non-linear, quasi-one-dimensional Euler equations modeling a flow in a variable-area stream tube $A(x)$ on a finite domain $x \in [0, 10]$.

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) &= -\frac{1}{A} \frac{dA}{dx} \rho u, \\
\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x} (\rho u^2 + p) &= -\frac{1}{A} \frac{dA}{dx} \rho u^2, \\
\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x} ([\rho E + p]u) &= -\frac{1}{A} \frac{dA}{dx} (\rho E + p)u,
\end{align*}
\]

where $\rho$ is the fluid density, $u$ is the fluid velocity, $p$ is the thermodynamic pressure, and $\rho E = \rho e + \frac{1}{2} \rho u^2$, is the total energy density. The pressure is related to $\rho E$ by the equation of state

\[ p = (\gamma - 1) \left( \rho E - \frac{1}{2} \rho u^2 \right), \]

for a perfect gas with ratio of specific heats $\gamma = 1.4$. The $x = 0$ boundary models a reservoir with specified total stagnation pressure $p_t = 101325 Pa$, and stagnation temperature $T_t = 300T$, while the right boundary at $x = 10$ enforces a specific static back pressure, $p_b = 73145$. The variable-area stream tube is defined as follows

\[ A(x) = 1.398 + \mu \tanh(1.8(x - 5)), \]

where $\mu \in [0, 1]$. Equation (4.1) is discretized using central finite differences and stabilized using a first-order artificial viscosity scheme. $N = 200$ grid points are used to discretize the domain $0 \leq x \leq 10$. The solution is marched to steady state using the implicit Euler time integration scheme.

Solution snapshots are computed using a fully Eulerian solver for 10 instances of the parameter $\mu_i = 0.1 + 0.13(i - 1)$, for $i = 1, \ldots, 10$. Lagrangian basis are constructed by solving the modified low-rank approximation problem, (3.5). As demonstrated in Fig. 5, the solution compressed using $k = 2$ Lagrangian basis is indistinguishable from the HFM, while the $k = 2$ Eulerian approximation contains large amplitude oscillations in the vicinity of the shock.

4.4. Computational speed-up

Solving (3.4), or (3.6) requires the computation of the projection of high-dimensional vectors and matrices on the reduced basis $U_x$ and $U_w$. The complexity of this computation scales with the size of the HFM, $N$. Therefore, while MOR reduces the size of the computational model from $N$ to $k$, part of the computational cost associated with solving the reduced problem still scales with the size of the HFM. For general nonlinear systems, an additional level of approximation is required to achieve the desired speed-up. During the last decade, several methods, occasionally referred to as “hyper-reduction” methods, have been developed for reducing the computational complexity of projection-based ROMs (Chaturantabut & Sorensen 2010, Carlberg et al. 2013, Farhat et al. 2015).
Figure 3: Model order reduction of scalar Burger’s equation with \( Re = 10^3 \); HFM (thick grey), \( k = 2 \) ROMs (dashed green), and \( k = 5 \) ROMs (solid red). Solutions are plotted for \( t = 0, 1/3, 2/3, 1 \).

Figure 4: ROM convergence for scalar convection-diffusion equation and Burger’s equation. Traditional Eulerian ROMs (dashed red lines with filled markers) and Lagrangian ROMs (solid black lines with empty markers).

Figure 5: The density along a converging/diverging nozzle, (5a): some different cases (\( \mu_1, \mu_5, \mu_{10} \)) comprising the snapshot matrix (5b): comparison of HFM (thick grey) and their reduced order representation in Eulerian (dashed blue) and Lagrangian (solid red) framework for \( \mu_{10} \) case.
The proposed method for the compression of solution snapshots characterized by moving sharp gradients is independent of the target projection-based MOR method. In particular, it is extendible to hyper reduction methods, but such an extension is beyond the scope of this paper.

5. Conclusions and future directions

A new Lagrangian projection-based model reduction approach has been introduced for the reduction of nonlinear, convection dominated flows. Global basis functions are used to approximate both the state and the location of the Lagrangian grid. In this framework, we demonstrate that certain wave-like solutions, or solutions characterized by moving shocks, discontinuities and sharp gradients exhibit low-rank structure and thus, admit efficient reduction using only a handful of global basis. The proposed approach was applied to several canonical one-dimensional problems for which the traditional Eulerian approach is known to fail. Lagrangian reduced order models are demonstrated to significantly outperform traditional, Eulerian-based reduced order models. An unexplored opportunity of our approach is the generalization to an arbitrary Lagrangian-Eulerian framework in order to avoid Lagrangian grid entanglement issues.

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