Model order reduction framework for problems with moving discontinuities

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Abstract We propose a new model order reduction (MOR) approach to obtain effective reduction for transport-dominated problems or hyperbolic partial differential equations. The main ingredient is a novel decomposition of the solution into a function that tracks the evolving discontinuity and a residual part that is devoid of shock features. This decomposition ansatz is then combined with Proper Orthogonal Decomposition applied to the residual part only to develop an efficient reduced-order model representation for problems with multiple moving and possibly merging discontinuous features. Numerical case-studies show the potential of the approach in terms of computational accuracy compared with standard MOR techniques.

1 Introduction

Hyperbolic partial differential equations (PDEs) are ubiquitous in science and engineering. Applications encompassing the fields of chemical industry, nuclear industry, drilling industry, etc., fall within this class. Model Order Reduction of systems of non-linear hyperbolic PDEs is a challenging research topic and is an active area of research in the scientific community. Moving discontinuities (such as shock-fronts) are representative features of this class of models and pose a major hindrance to obtain effective reduced-order model representations [1]. As a result, standard MOR techniques [2] do not fit the requirements for real-time estimation and control or multi-query simulations of such problems. This motivates us to investigate and pro-

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pose efficient, advanced and automated approaches to obtain reduced models, while still guaranteeing the accurate approximation of wave propagation phenomena.

A lot of research is in progress to improve the state of the art of MOR for transport-dominated problems: *(i)* (data-based and model-based) time and space-dependent coordinate transformation/ symmetry reduction framework [3, 4, 5, 6, 7, 8], *(ii)* optimal transport [9, 10, 11], *(iii)* interpolation/ dictionary/ tracking framework [12, 13, 14], *(iv)* adaptive and stabilization strategies [15, 16], and, *(v)* deep learning/ neural network concepts [17, 18]. These works have mainly focused on resolving transport along a single direction [3] and multiple directions [4] for linear and non-linear classes of (parameterized) problems.

Effective reduction of non-linear transport-dominated problems in the context of multiple moving (and merging) discontinuous features is still challenging. Few notable works that aim at mitigating this problem are [12, 13, 4]. The works [12, 13] are based on the concept of (low and high resolution) transformed snapshot interpolation. Such an approach has been particularly tested in the regions near (and at) the singularity, induced upon merging of the wavefronts. Another work in this direction is the concept of freezing multiple frames [19]. However, their performance, demonstrated for parabolic problems, does not carry over to less regular hyperbolic problems and suffers from additional travelling structures or numerical instabilities in the decomposed components. Moreover, the existing methods [4, 19] lack the (online-efficient) automated identification of switching point from multiple wavefront setting to single wavefront setting upon merging of wavefronts.

We propose an approach that is a stepping stone towards resolving the aforementioned issues. The main contribution of the work is to propose a new decomposition ansatz that decomposes the solution into a basis function that tracks the evolving discontinuity and a residual part that is expected to be devoid of shock features. This decomposition renders the residual part to be amenable for reduced-order approximation. We, then, use these generated bases to apply Proper Orthogonal Decomposition (POD) on the residual part and later reconstruct the solution by lifting it to the high-dimensional problem space. We finally assess the combined performance of decomposition, reduction and reconstruction approach (as opposed to conventional reduction and reconstruction approach) in the scope of transport-dominated problems with moving and interacting discontinuities.

2 Mathematical Formulation

We consider a scalar 1D conservation equation of the form:

$$\partial_t u(x,t) + \partial_x f(u(x,t)) = 0, \quad u(x,0) = u_0(x). \tag{1}$$

We assume that $u(x,0) = u_0(x)$ already has S number of discontinuities at locations $x_1(0), \ldots, x_S(0)$ with values $u^-(x_s(0),0), \quad s = 1,\ldots,S$ from the left and values $u^+(x_s(0),0), \quad s = 1,\ldots,S$ from the right. We associate a single basis function

$\sigma_s(x - x_s(t))$ to each discontinuity at their respective locations. This basis function has a jump of height 1, i.e., $\sigma_s^+(0) - \sigma_s^-(0) = 1$, at the location of the discontinuity and can have any (preferably continuous and smooth) shape away from the discontinuity.

We now decompose the solution of (1) in the following way:

$$u(x,t) = \sum_{s=1}^{S} j_s(t)\sigma_s(x - x_s(t)) + u_r(x,t),$$

$$j_s(t) = u^-(x_s(t),t) - u^+(x_s(t),t). \tag{2}$$

If $x_s(t)$ exactly matches the shock locations and (2) is exactly fulfilled, then $u_r(x,t)$ does not contain any discontinuities and is amenable to a low-rank approximation.

The time-stepping scheme is defined in the following way. In each time step, we:

- Compute updated shock locations $x_s(t^{n+1})$ using the Rankine Hugoniot condition.
- Compute $u^{\pm}(x_s(t^{n+1}),t^{n+1})$ in a neighborhood of $x_s(t^{n+1})$ and define jumps, $j_s(t^{n+1})$, via (2).
- Compute the residual part $u_r(x,t^{n+1})$ from

$$u_r(x,t^{n+1}) - u_r(x,t^n) = \sum_{s=1}^{S} j_s(t^n)\sigma_s(x - x_s(t^n)) - \Delta t \partial_x f(u(x,t^n)) - \sum_{s=1}^{S} j_s(t^{n+1})\sigma_s(x - x_s(t^{n+1})). \tag{3}$$

The standard way to construct a reduced-order model (ROM) is to reduce (1) by applying Galerkin projection on u. Instead, we reduce (3) via Galerkin projection onto $V_N \subseteq V_h$, where V_N is a N-dimensional reduced space spanned by the functions obtained from a truncated singular value decomposition of the u_r snapshot matrix, and V_h is a h-dimensional high-fidelity space. Upon considering the projection operator $P_N : V_h \to V_N$, the reduced scheme takes the following form:

$$u_{r,N}^{k+1} = u_{r,N}^k + P_N\Big(\sum_{s=1}^{S} j_{s,N}(t^k)\sigma_s(x - x_{s,N}(t^k)) - \Delta t \partial_x f(P_N^{'} u_N^k) - \sum_{s=1}^{S} j_{s,N}(t^{k+1})\sigma_s(x - x_{s,N}(t^{k+1}))\Big), \tag{4}$$

where $u_{r,N}^k \in V_N$ and $u_{r,N}^0 = P_N(u_r^0)$ with u_N^k defined in the following form:

$$P_N^{'} u_N^k = \sum_{s=1}^{S} j_{s,N}(t^k)\sigma_s(x - x_{s,N}(t^k)) + P_N^{\prime} u_{r,N}^k, \tag{5}$$

and, $j_{s,N}$ and $x_{s,N}$ are, respectively, the jumps and shock locations computed during the ROM time-stepping. $j_{s,N}$ and $x_{s,N}$ can be obtained in a manner similar to the steps carried out during the full-order model (FOM) time-stepping.

It is well known that projection alone is not sufficient to reduce the costs of computing the solution of a reduced-order model if the Finite Volume operators are non-linear in nature. Empirical Operator Interpolation [20] can be used here as a recipe for hyper-reduction. We do not delve into the full and efficient offline and online decomposition as its discussion is not within the scope of this work. However, we mention that we need to know $j_{s,N}(t^k)$ and $u_{r,N}(x_{s,N}(t^k), t^k)$ for computing $x_{s,N}(t^{k+1})$. In a reduced scheme this means that we need to keep the entire reduced basis in memory. However, the basis vectors are only evaluated at the shock locations at each time step. The same consideration holds for the computation of the $j_{s,N}(t^{k+1})$.

3 Numerical Experiments

We numerically test the new approach and show its potential as a reduced-order modelling technique. We reduce Burgers equation, which is given by:

$$\partial_t u + \partial_x(\frac{u^2}{2}) = 0, x \in [0, L]. \tag{6}$$

The case studies consider that the shock is already present in the initial data, which for single and multiple wavefront scenarios, is respectively given by:

$$u(x,0) = u_0(x) = \begin{cases} x, & 0 \le x \le 1, \\ 0, & \text{otherwise} \end{cases} \quad \text{and} \quad u(x,0) = u_0(x) = \begin{cases} x-2, & 2 \le x \le 4, \\ \frac{(x-5)}{2}, & 5 \le x \le 7, \\ 0, & \text{otherwise.} \end{cases}$$

We consider only periodic boundary conditions. Furthermore, we consider the spatial domain to be $L = 10$ and use an upwind finite volume (FV) scheme for the spatial discretization and first-order Forward Euler for the time-stepping. We take 8000 steps in time for the scenarios under consideration i.e., $t \in [0, 4]$ with a timestep of 0.0005. We consider three different spatial mesh resolutions (spatial step size of 0.005, 0.002 and 0.001) to assess the performance of the standard (POD without decomposition) and the proposed approach.

We quantify the performance of the standard and the proposed approach by computing the reduced-order modeling (ROM) error. We consider L^2 in space and L^2 in time (absolute) error and define it in the following manner (for a basis-size N):

$$e_{rom} = \sqrt{\Delta t \sum_{k=1}^{N_T+1} \Delta x \sum_{i=1}^{N_x} \mid u_{i,k} - (P'_N u_N^k)_{i,k} \mid^2}. \tag{7}$$

where Δt is the time-step, Δx is the spatial step, N_T is the number of time-steps and N_x is number of Finite Volume elements. $u_{i,k}$ means u at $x = x_i$ and $t = t_k$ (similarly for $(P'_N u_N^k)_{i,k}$). Herewith, (7) expresses the error between the full-order model (Finite Volume solution) governed by (1) and the reconstruction given by (5)).

3.1 Single wavefront scenario

We first consider the scenario where only a single discontinuous front evolves across the spatial domain. Here, we use the following shape function for $\sigma_s(x - x_s)$:

$$\sigma_s(x - x_s) = \begin{cases} 1 + x - x_s, & x_s - 1 \le x \le x_s, \\ 0, & \text{otherwise.} \end{cases}, \quad s = 1, .., S, \tag{8}$$

with $S = 1$, $x_s(t = 0) = 1$.

3.2 Multiple wavefront scenario

Here, we consider the setting where multiple (discontinuous) wavefronts evolve across the spatial domain and also interact non-linearly with each other. We study the scenario where two wavefronts are present in the spatial domain and the left front propagates faster than the right one. We, however, restrict the study to only assess the performance of the proposed approach in dealing with the interaction of the head of one wavefront with the tail of the other one. We postpone the discussion of automatically dealing with the merging of wavefronts for future work. We use the following shape function for $\sigma_s(x - x_s)$ to study this scenario.

$$\sigma_s(x - x_s) = \begin{cases} 1 + \frac{1}{2}(x - x_s), & x_s - 2 \le x \le x_s, \\ 0, & \text{otherwise} \end{cases}, \quad s = 1, .., S, \tag{9}$$

with $S = 2$, $x_{s=1}(t = 0) = 4$ and $x_{s=2}(t = 0) = 7$.

3.3 Discussion

Interpolation of $\sigma_s(x - x_s(t))$ onto the FV mesh results in numerical approximation error. As a result, we observe residual jumps in the residual part, u_r, during FOM simulation. The aim is to build a reduced space by applying POD on the residual part. One option could be to build the bases (or reduced space) from the computed residual part (with residual jumps). An other alternative could be to post-process the residual part (computed during FOM) in order to get rid of the residual jumps. This post-processed residual part, which is even more low-rank approximable than the residual part with residual jumps, can be then used to build the (effective) reduced space. We invoke one of these ways to generate the bases and build a ROM.

We, first, consider the setting where the shock locations and jumps computed during FOM simulation are used during the ROM time-stepping i.e., we assume that $j_{s,N} = j_s$ and $x_{s,N} = x_s$. We, further, use the computed residual part (with residual jumps) to generate the bases. We can clearly see the benefits of the proposed approach in Figure 1, which shows the behavior of the ROM error for increasing basis sizes N across different mesh resolutions. Firstly, the initial error incurred via the proposed approach is clearly lower than that of the standard approach. This is attributed to the fact that our decomposition approach associates a basis function corresponding to the travelling discontinuity. Secondly, the rate of decay of the error is better for the proposed approach compared to the standard approach. We also see that the ROM error for the standard approach is larger for finer mesh-sizes. This occurs as the effect of the shock becomes more pronounced for finer meshes. Also, the finer mesh implies less numerical viscosity. We also observe that the ROM errors could even increase with an increment in the basis size. It can be argued that this could occur as a result of insufficiently many basis functions. However, the ROM error for the proposed approach decreases with an increment in basis size. Moreover, the ROM error is lower (and stagnates later) for finer mesh-sizes. This can be argued from the fact that the proposed approach is able to resolve the shock more accurately at finer meshes. This error behavior is clearly in contrast to that of the standard approach which fails to efficiently capture the shock. As a result, the difference between the ROM error (at a certain number of basis function) computed via standard and proposed approach becomes even more pronounced for finer meshes.

Figure 2 demonstrates the performance for fully ROM computations, i.e., shocks locations, $x_{s,N}$ and jumps, $j_{s,N}$ are computed during ROM time-stepping. We perform post-processing on the residual part computed during FOM. u_r is post-processed by linear interpolation between the locations x_s^+, x_s^- where the local minimum u^+ and maximum u^- in a neighborhood of x_s is attained. We, then, generate the bases from this post-processed residual part. The post-processing was not needed in an earlier setting (discussed in the paragraph above) as accurate shock locations and jumps from the FOM simulation were used. However, it becomes essential here in order to approximate $x_{s,N}$ and $j_{s,N}$ within the ROM time-stepping with good accuracy. We observe that the proposed approach still performs better than the standard approach. However, the proposed approach seems to incur larger ROM error for

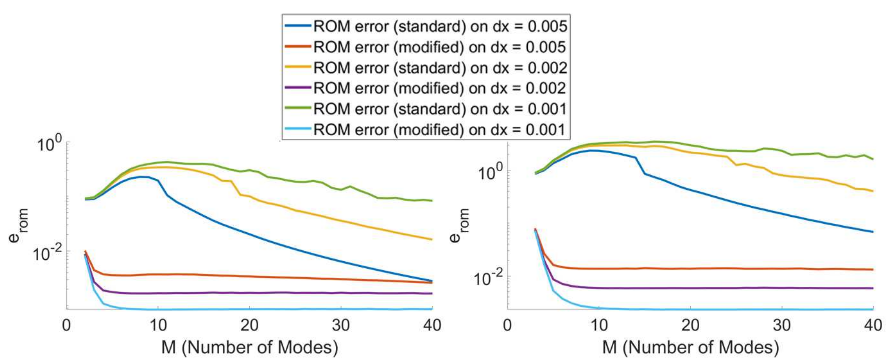

Fig. 1 ROM error upon using shock locations and jumps computed during FOM simulation: (left) single wavefront scenario and (right) multiple wavefront scenario.

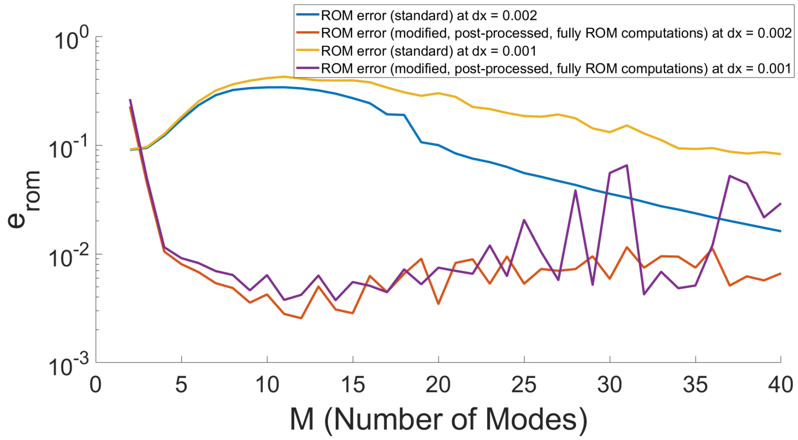

Fig. 2 ROM error under fully ROM computations for the single wavefront scenario.

larger POD mode numbers. Similar issues (not included in this paper) are observed for the multiple wavefront scenario. Such issues did not exist when we used the shock locations and jumps from FOM during the ROM time-stepping. Hence, the issues could be caused from a poor approximation of the shock. A possible explanation could be that we have more oscillations (around the shock position in the residual part) as the number of POD modes increases. The oscillations, which appear due to the reduced regularity of the residual part, lead to wrong computation of $x_{s,N}$ and $j_{s,N}$. It is clear that $x_{s,N}$ (and $j_{s,N}$) need to be approximated with good accuracy. The error in $x_{s,N}$, which would increase over time, should be in the order of the discretization error to achieve an overall ROM error in the order of the discretization error. A mitigating measure could be to improve shock approximation similar to [14]. The high-frequency modes could also be a source of the problem. The potential solution could be to filter out the high-frequency modes when advancing the shock.

4 Conclusions

We have proposed a decomposition ansatz and used it in conjunction with POD. We have show-cased the performance of the proposed approach on the Burgers equation. The proposed approach is able to resolve the discontinuities and also offers reduction in ROM error. Future work will deal with resolving issues that exist in the proposed approach for larger POD mode numbers. Moreover, we will adapt the discussed formulation for system of conservation laws. We will also assess the performance of the method for parametrized scalar and system of conservation laws.

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