Implementation of Manifold-Based Combustion Models in a Highly Scalable Low Mach Number Reacting Flow Solver

Preprint

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Implementation of Manifold-Based Combustion Models in a Highly Scalable Low Mach Number Reacting Flow Solver

Bruce A. Perry[1,*], *Marc T. Henry de Frahan*[1], *Shashank Yellapantula*[1], *and Marc S. Day*[1]

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Abstract: Manifold-based representations of the thermochemistry are often employed in conjunction with large eddy eimulation (LES) to lower the cost of combustion simulations. This work describes steps taken to implement this modeling approach in PeleLM, a scalable and performance-portable low Mach number flow solver. Most significantly, this includes adapting the projection method used by PeleLM to satisfy the mass conservation constraint for use with manifold-based models. The implementation is designed to be general across manifold-based models, including both those that employ traditional tabulation and those that employ neural networks. An initial demonstration for simple test cases is presented and will be used for performance assessment.
Keywords: Large Eddy Simulation, High-Perfromance Computing, Reduced-order Manifolds

1. Introduction

The Pele suite of codes[1] is a set of combustion application tools being developed as part of the United States Department of Energy's Exascale Computing Project with the aim of enabling high-fidelity simulations of realistic combustion configurations. These simulations will be run on a variety of computing platforms, including next-generation computing architectures. The suite of codes includes a compressible solver (*PeleC*), a low Mach number solver (*PeleLM*), and a shared physics library (*PelePhysics*), and has thus far been primarily targeted toward well-resolved simulations with detailed chemical mechanisms [1, 2]. However, the broad class of manifold-based combustion models, often coupled with Large Eddy Simulation (LES), reduces the cost of turbulent combustion simulations and it is also desirable to run simulations at large-scale using these models. Therefore, the present work focuses on adaptation of PeleLM and PelePhysics to enable use of manifold-based models. First, we describe the general category of models covered by the implementation, which is designed to cover most manifold-based models. Next, we discuss the algorithmic modifications required for the low Mach number solver, which is then demonstrated using a wrinkled premixed flame and a multispecies advection-diffusion problem as test cases.

[1] https://github.com/AMReX-Combustion

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2. Manifold-Based Models

The key principle behind all manifold-based models is that the thermochemical states within most combustion systems tend to evolve approximately on a low dimensional manifold within the thermochemical state space (defined all species mass fractions, temperature, and pressure) [3]. The cost of simulations can be greatly reduced by solving equations for quantities that parameterize the manifold rather than the for all of the species, and applying a function that maps from these parameters to the composition, reaction rates, transport coefficients, and any other thermochemical quantities of interest. In physically-derived models, like flamelet-based models [4, 5], the manifold and mapping function are constructed by tabulating solutions to one-dimensional flames or other simple computations as a function of physical quantities like the mixture fraction, reaction progress variable, and their dissipation rates. Manifolds may also be defined empirically from data, for example using principal component analysis (PCA) [6], which gives parameters based on linear combinations of species. In either case, neural networks may be used to replace tabulation for the mapping [7, 8], and approaches that use neural networks for the entire manifold-based modeling process also show significant promise [9]. Finally, for closure when used with LES, the subfilter (co)variances of the manifold parameters may be used to aid in tabulated closure of filtered thermochemical variables.

All of the models described above can be summarized as providing a relationship of the form:

$$\widetilde{\phi}_n = \mathscr{G}_n(\widetilde{\xi}_i, \sigma_{jk}, \widetilde{\alpha}_m, p) \tag{1}$$

where $\widetilde{\phi}_n = [\bar{\rho}, \widetilde{\mu}, \widetilde{D}, \widetilde{T}, \bar{\omega}, ...]$ includes any filtered thermochemical quantity of interest, $\widetilde{\xi}_i$ is the vector of manifold parameters for which scalar transport equations are solved, $\sigma_{jk} = \widetilde{\xi_j \xi_k} - \widetilde{\xi}_j \widetilde{\xi}_k$ is the subfilter covariance matrix of these parameters (also obtained by solving a scalar transport equation), $\widetilde{\alpha}_m$ is the vector of any algebraically computed parameters (e.g., scalar dissipation rate), and the function $\mathscr{G}_n$ is provided in the form of a table or neural network. Note that the thermodynamic pressure p corresponding to the data used to generate the manifold has been explicitly added as a parameter, though it is a constant value for low Mach number flows in open systems. Typically, only a subset of the input parameters are included for any given model, but the full set is considered in this work and the manifold is allowed to have an arbitrary number of dimensions to ensure a general implementation.

3. Numerical Approach

PeleLM uses a block structured grid with adaptive mesh refinement (AMR) through the AMReX library [10] and an embedded boundary treatment to handle complex geometries. The numerical approach is based on the projection approach developed by Almgren et al. [11] and adapted for combustion by Day and Bell [12] and Nonaka et al. [13]. The key part of this algorithm is the projection of the velocity field onto a constraint surface where the divergence of the velocity field satisfies the continuity equation. A full description of the algorithm is beyond the scope of this abstract, but may be found in the code documentation[2]. The key aspects of the algorithm and its existing implementation are depicted in Fig. 1. The spectral deferred correction (SDC) iteration

[2] `https://amrex-combustion.github.io/PeleLM/manual/html/index.html`

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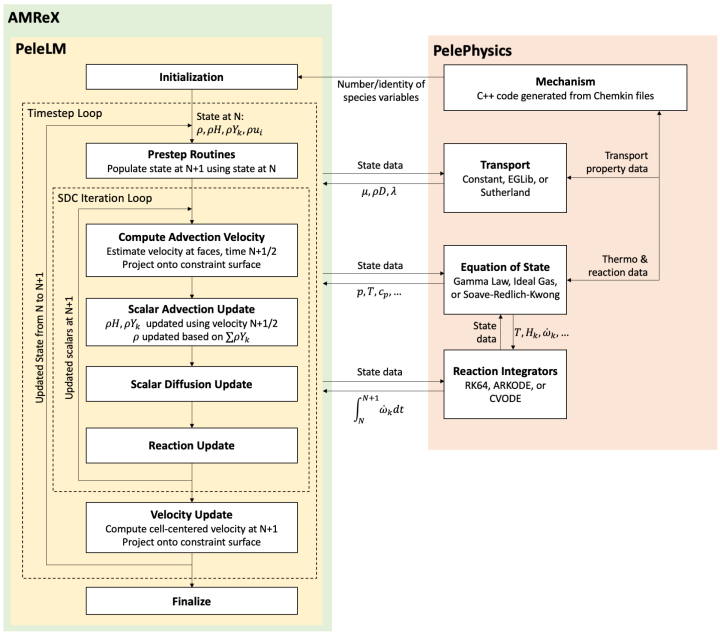

Figure 1: Simplified schematic of the existing PeleLM solution algorithm, showing the relationship of the involved codes.

loop tightly couples the multi-physics scalar advance even though advection, diffusion, and reaction are treated separately. PelePhysics contains polymorphic classes for computing transport properties, the equation of state (EOS) and other thermodynamic properties, and integrating reactions within each timestep to account for stiffness, allowing for different models and functionality to be called upon for these purposes as needed in PeleLM.

The adapted implementation for manifold-based simulations is shown in Fig. 2. On the PeleLM side, the main difference is in the transported state quantities, which now include the filtered manifold parameters and their subfilter variances instead of the enthalpy and species. Because these quantities follow similar transport equations to the species, minimal algorithmic changes to PeleLM are needed. One notable change is that density is advected based on the sum of species densities to ensure consistency for the case with full chemistry, but for the manifold case $\sum \bar{\rho} \widetilde{\xi}_i \neq 1$, so density is advected independently. A significant difference is that, though the procedure is otherwise equivalent, the constraint on the divergence of the velocity is computed differently for the manifold case. There are notable structural changes on the PelePhysics side, where new EOS and transport classes wrap around a new class that provides the ability to evaluate the nonlinear mapping function for the manifold model, rather than evaluating analytical functions based on mechanism data. This modular structure is designed to allow for different manifold-based modeling approaches to be easily implemented, whether they rely on traditional tabulation or neural networks.

An important development required to implement manifold-based models is reformulation of the divergence constraint developed for combustion with detailed chemistry by Day and Bell [12].

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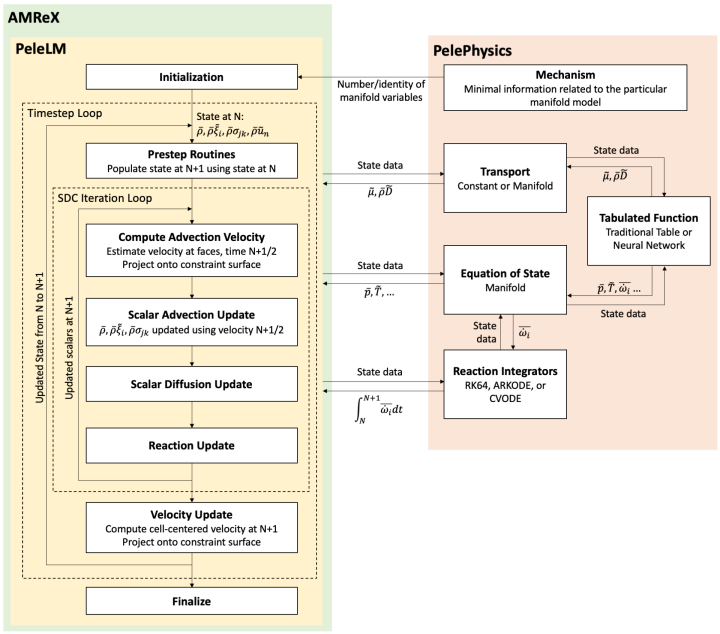

Figure 2: Simplified schematic of the modified PeleLM approach for manifold-based combustion models, showing the relationship of the involved codes.

In that case, the constraint on the velocity field can be written

$$\begin{aligned}\frac{\partial u_j}{\partial x_j} = \frac{-1}{\rho}\frac{D\rho}{Dt} &= \frac{-1}{\rho}\left[\frac{\partial \rho}{\partial p}\frac{Dp}{Dt} + \frac{\partial \rho}{\partial T}\frac{DT}{Dt} + \sum_k \frac{\partial \rho}{\partial Y_k}\frac{DY_k}{Dt}\right] \\ &= \frac{1}{T}\frac{DT}{Dt} + W\sum_m \frac{1}{W_k}\frac{DY_k}{Dt},\end{aligned} \tag{2}$$

where the low Mach number approximation ($Dp/Dt = 0$) has been applied and the ideal gas equation of state ($p = \rho RT$) has been used to simplify the partial derivatives. The evolution equations for T and Y_k can then be substituted and the constraint evaluated. While this approach can be extended to non-ideal equations of state [14], it cannot be directly applied when transport equations for the species are not solved. An alternative approach is to use the chain rule to expand the material derivative of density not based on thermodynamic variables, but based on the manifold parameters:

$$\begin{aligned}\frac{\partial \widetilde{u}_j}{\partial x_j} = \frac{-1}{\bar{\rho}}\frac{D\bar{\rho}}{Dt} &= \frac{-1}{\bar{\rho}}\left[\frac{\partial \mathscr{G}_0}{\partial p}\frac{Dp}{Dt} + \sum_n \frac{\partial \mathscr{G}_0}{\partial \widetilde{\xi}_i}\frac{D\widetilde{\xi}_i}{Dt} + \sum_q \frac{\partial \mathscr{G}_0}{\partial \widetilde{\alpha}_m}\frac{D\widetilde{\alpha}_m}{Dt} + \sum_m\sum_n \frac{\partial \mathscr{G}_0}{\partial \sigma_{jk}}\frac{D\sigma_{jk}}{Dt}\right] \\ &= \frac{-1}{\bar{\rho}}\left[\sum_n \frac{\partial \mathscr{G}_0}{\partial \widetilde{\xi}_i}\frac{D\widetilde{\xi}_i}{Dt} + \sum_q \frac{\partial \mathscr{G}_0}{\partial \widetilde{\alpha}_m}\frac{D\widetilde{\alpha}_m}{Dt} + \sum_m\sum_n \frac{\partial \mathscr{G}_0}{\partial \sigma_{jk}}\frac{D\sigma_{jk}}{Dt}\right].\end{aligned} \tag{3}$$

In this case, analytical expressions for the partial derivatives are not available, but they be easily evaluated using finite differences if $\mathscr{G}$ is encoded using a traditional table, or using functionality standard in machine learning libraries if $\mathscr{G}$ is encoded using a neural network. While known

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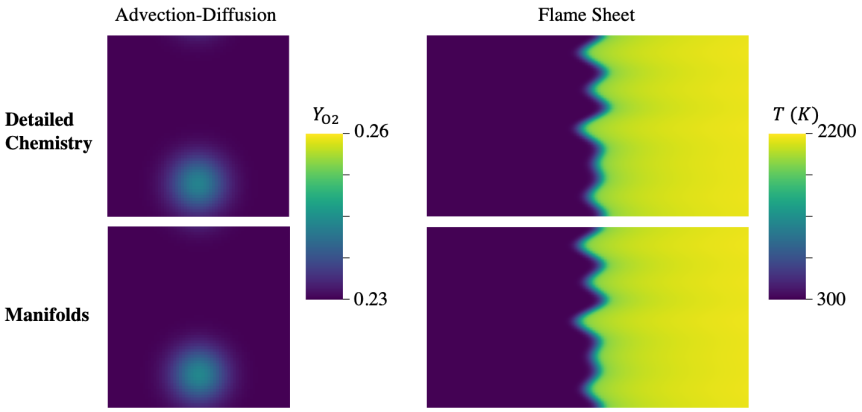

Figure 3: Qualitative comparison between manifold-based solution and detailed chemistry solution for two simple test cases using PeleLM

transport equations allow the $\widetilde{\xi}_i$ and σ_{jk} terms to be directly evaluated, because $\widetilde{\alpha}_m$ are computed algebraically, that term cannot be evaluated. Therefore, the implementation is presently limited to models without algebraic parameters, with approaches to resolve this left as future work.[3]

4. Demonstration

A simple two-species advection-diffusion problem and a wrinkled two-dimensional premixed methane-air flame with DRM19 chemistry were chosen to validate the manifold model implementation, as it should be able to recover the detailed chemistry behavior in both cases without modeling error. For simplicity, both cases are fully resolved (subfilter variances are not included) and rely on one-dimensional manifolds: one-dimensional mixing parameterized by a mixture fraction for the advection-diffusion case and a one-dimensional premixed flame parameterized by progress variable for the wrinkled flame case. As shown in Fig. 3, the manifold-based approach correctly yields equivalent predictions to the full solution with detailed chemistry. Significant performance gain ($\sim$ 4 times speed-up) was observed, but further assessments will evaluate the performance gains obtained by using the manifold-based approach in more detail.

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[3]One possibility is that the correction procedure developed by Nonaka et al. [13] to ensure numerical error does not lead to deviation from the equation of state can also compensate for error induced by neglecting this term.

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References

[1] H. Sitaraman, S. Yellapantula, M. T. H. de Frahan, B. Perry, J. Rood, R. Grout, and M. Day, Adaptive mesh based combustion simulations of direct fuel injection effects in a supersonic cavity flame-holder, Combust. Flame 232 (2021) 111531.

[2] H. Sitaraman, N. Brunhart-Lupo, M. H. de Frahan, S. Yellapantula, B. Perry, J. Rood, R. Grout, M. Day, R. Binyahib, and K. Gruchalla, Visualizations of direct fuel injection effects in a supersonic cavity flameholder, Physical Review Fluids 6 (2021) 110504.

[3] S. B. Pope, Small scales, many species and the manifold challenges of turbulent combustion, Proc. Combust. Inst. 34 (2013) 1–31.

[4] C. D. Pierce and P. Moin, Progress-variable approach for large-eddy simulation of non-premixed turbulent combustion, J. Fluid Mech. 504 (2004) 73–97.

[5] J. Van Oijen, R. Bastiaans, and L. De Goey, Low-dimensional manifolds in direct numerical simulations of premixed turbulent flames, Proc. Combust. Inst. 31 (2007) 1377–1384.

[6] J. C. Sutherland and A. Parente, Combustion modeling using principal component analysis, Proc. Combust. Inst. 32 (2009) 1563–1570.

[7] M. Ihme, C. Schmitt, and H. Pitsch, Optimal artificial neural networks and tabulation methods for chemistry representation in LES of a bluff-body swirl-stabilized flame, Proc. Combust. Inst. 32 (2009) 1527–1535.

[8] M. R. Malik, B. J. Isaac, A. Coussement, P. J. Smith, and A. Parente, Principal component analysis coupled with nonlinear regression for chemistry reduction, Combust. Flame 187 (2018) 30–41.

[9] B. A. Perry, M. T. Henry de Frahan, and S. Yellpantula, Co-Optimized Machine-Learned Manifold Models for Large Eddy Simulation of Turbulent Combustion, Combust. Flame (2022) under review.

[10] W. Zhang, A. Myers, K. Gott, A. Almgren, and J. Bell, AMReX: Block-structured adaptive mesh refinement for multiphysics applications, The International Journal of High Performance Computing Applications (2021) 10943420211022811.

[11] A. S. Almgren, J. B. Bell, P. Colella, L. H. Howell, and M. L. Welcome, A conservative adaptive projection method for the variable density incompressible Navier–Stokes equations, J. Comp. Phys. 142 (1998) 1–46.

[12] M. S. Day and J. B. Bell, Numerical simulation of laminar reacting flows with complex chemistry, Combustion Theory and Modelling 4 (2000) 535.

[13] A. Nonaka, M. S. Day, and J. B. Bell, A conservative, thermodynamically consistent numerical approach for low Mach number combustion. Part I: Single-level integration, Combustion Theory and Modelling 22 (2018) 156–184.

[14] J. Bell, M. Day, C. Rendleman, S. Woosley, and M. Zingale, Adaptive low Mach number simulations of nuclear flame microphysics, J. Comp. Phys. 195 (2004) 677–694.

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