



Dual-time schemes for reacting flows with stiff kinetics

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ABSTRACT

Two operator-split schemes designed for handling stiff chemistry are proposed within a dual-time framework and tested using zero- and one-dimensional test problems. Both are shown to perform robustly without *ad hoc* time-step restrictions. The first scheme is a Physical Splitting Scheme that is a straightforward extension of the Strang splitting method. Like the Strang splitting method, it retains the issue of splitting errors degrading solution accuracy at large time steps. However, it performs well at small time-steps and remains competitive because the scheme involves only two ODE solutions per physical time step. The second scheme is the Consistent Splitting Scheme that is designed to eliminate the splitting errors, but is relatively more expensive because it requires two ODE solutions per pseudo-time step. This scheme also performs well at small to moderate time steps, but its accuracy also degrades at large time steps in part because of issues associated with finite precision. This study indicates the relative strengths and weaknesses of operator splitting approaches and points the way for continued research.

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1. Introduction

Advances in computational power enable simulations of increasingly complex turbulent, reacting flows. Many of these reacting flows have a wide range of spatial and temporal scales that dictate the physical models and numerical schemes required for proper simulation. Some of the time-scales arise directly from the fluid-mechanics such as particle convective speeds, diffusion velocities, and acoustic scales, which can be widely disparate or stiff at low Mach numbers and in high-Reynolds number boundary layer regions. In reacting flows, chemical reaction time scales are often faster than even the fastest fluid time scales, which are typically the acoustic scales, leading to additional time-scale disparities. This is especially the case for systems wherein detailed chemical kinetics are needed, for instance, transient phenomena such as ignition, extinction, or low-temperature fuel oxidation are important, or systems where radical production or pollutant production is important. The detailed chemical mechanisms are generally stiff and radicals evolve rapidly, often faster than the largest stable time steps of explicit schemes, and require special treatment

for the chemical source terms [1–10]. In this work, we explore issues related to stiff chemistry in the context of the so-called dual-time scheme, which is the framework we adopt to handle the stiffness due to fluid mechanics [11–13].

A well-established density-based compressible algorithm for addressing the stiffness due to the convective and acoustic time scales for low Mach number flows is the preconditioning method, wherein a set of pseudo-time derivatives are used to condition the system to obtain proper accuracy and efficiency [11–13]. For time-accurate flows, the preconditioned scheme is implemented within a dual-time framework with distinct sets of physical and pseudo-time derivative terms. This allows a high-order scheme to be used for the physical-time derivative, with the second-order accurate, backward different formula being the common choice due to its unconditional stability. Within each physical time-step, the pseudo-time derivatives are marched forward until it reaches a “steady-state”, at which point the physical solution for the next time step is attained. We point out that any time marching scheme may be used to drive the pseudo-time integration, including both implicit and explicit schemes. Due to the inherently non-physical nature of the pseudo-time derivative, various acceleration techniques that would otherwise destroy time accuracy can be used, including local time stepping, multigrid acceleration, as well as the low-Mach number preconditioning mentioned earlier. Thus, in addition to acoustic-wave stiffness, grid-induced stiffness due

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to the use of high-aspect ratio cells in high-Reynolds number boundary layers can also be efficiently tackled. In other words, the fundamental advantage of the dual-time framework is that it allows the physical time-step selection to be made based purely on physical considerations irrespective of numerical stability considerations, which are handled optimally by the pseudo-time integration process.

For chemically reacting flows, dual-time schemes are usually implemented in a fully coupled fashion, where the source terms and spatial terms are treated together using the pseudo-time iterator [11,14–16]. However, there are no established approaches for treating stiff chemical mechanisms. This represents the motivating objective of the present study. We start by reviewing methods for handling chemical stiffness in general, including ordinary differential equations and single-time reacting-fluid systems, and use this understanding to explore the underlying issues and to develop methods within the dual-time framework.

The time scales of the chemical mechanism are determined by the eigenvalues of the Jacobian matrix associated with the mechanism and the stiffness is quantified by the ratio of the magnitudes of the largest to the smallest eigenvalues. We note for clarity that the time scales of the mechanism are, in fact, the inverse of the magnitude of the real component of the eigenvalues. When the chemical integration is treated numerically, stiffness generally requires implicit treatment for efficient convergence to the solution. However, eigenvalues with large, positive, real components are destabilizing for an implicit scheme [11,14] and reduce the permissible step sizes. The computational singular perturbation (CSP) technique indicates that positive eigenvalues are largest through pre-heat and reaction fronts, but may remain post-flame [17–19]. CSP also shows a wide range of magnitudes for the eigenvalues, even post-flame. Therefore, the system remains stiff and implicit schemes are desirable, but the positive eigenvalues reduce the effectiveness of the implicit integration.

Reduction of the stiffness in the chemical source terms in ordinary differential equations (ODE) encountered in zero-dimensional reactor problems has been achieved using multiple techniques. The most popular of these methods are based on implicit methods for sparse systems. Numerous solvers exist and combine information contained in the eigenvalues with careful selection of the time step size to control the error and minimize the stiffness of the problems. A popular example is the DVODE solver [20].

Integration of chemical source terms for the partial differential equations representing reacting flows have been formulated for single-time schemes. Broadly speaking, two different approaches have been used. The first is a fully-coupled approach, where the chemical source terms are integrated alongside the spatial terms using the same temporal integrator. These schemes rely on the temporal integrator to address the stiffness and time step limitations due to the source terms. For implicit temporal schemes, the stiffness is addressed automatically for negative eigenvalues by the scheme's unconditional stability, but the presence of eigenvalues with large, positive components limits the time step selection. For explicit temporal schemes, the eigenvalues with positive, real components do not impose any linear stability constraints, although non-linear constraints remain. However, the eigenvalues with negative, real components impose significant time step constraints for stability, and for stiff systems, the time-step sizes can be prohibitively small [11].

Several researchers have proposed advanced techniques to handle stiffness within a fully coupled, single-time framework. The dynamic adaptive hybrid integration (AHI) approach integrates the fast species and reactions using an implicit scheme while the slow reactions are integrated using an explicit scheme [10]. By removing the slow species from the system requiring implicit integration,

the size of the source term Jacobian is significantly reduced and in turn, the cost of the implicit solver is also reduced. Other efforts to control the implicit treatment are due to Katta and Roque-more [21] and Savard et al. [22], wherein approximate source Jacobians are used to cast the problem as a semi-implicit procedure to accelerate the performance. These developments have hitherto been implemented within a pressure-split fluid mechanics algorithm, rather than the fully-coupled, density-based method that is the focus here. Sankaran and Oefelein [23] presented a preconditioning method for integrating stiff chemical mechanisms. The authors attempt to derive a scaling parameter for a global mechanism, which modifies the eigenvalues of the reacting system by turning the large, positive eigenvalue into a negative eigenvalue, thereby stabilizing it. More recent work by Hansen and Sutherland [24] extends this work for more complex chemical mechanisms. These efforts for preconditioning the source term integration are still confined to zero-dimensional reactors and have not yet been applied to multi-dimensional reacting flows. Overall, *ad hoc* strategies are still needed to adequately control the stability and accuracy of such methods.

The second approach is to treat the chemical source terms as a local, point-wise problem decoupled from the spatial fluxes. These are known as operator splitting, or fractional step, methods and permit the use of dedicated solvers for solving the stiff chemical source term differential equations that arise within each computational point [2,25–28]. Such solvers are optimized for treating the disparate scales that arise in detailed kinetics.

While the operator splitting approach segregates the workload into highly efficient, dedicated solvers, the approach introduces splitting errors due to the decoupling of the source terms and the spatial fluxes [4]. Depending on the precise splitting scheme chosen, these errors have various leading order of truncation errors. Strang splitting is a popular choice and these splitting errors are formally second-order accurate [1,4,6]. The truncation error, however, also depends upon the Jacobian of the source term and hence on its eigenvalues. This means that, despite the formal order of accuracy, the actual magnitude of the splitting error may be large, especially for stiff systems. Therefore, these schemes also require special treatment to ensure the steady state solution is the same as the unsplit scheme [29].

Schwer et al. [5] have formulated a consistent-splitting scheme in the context of a single-time, steady-state formulation by recognizing that the source of the splitting error is the inconsistent choice of residual equation in the chemistry and fluids integration step. In the consistent scheme, they implement an alternative splitting algorithm wherein both the chemistry and fluid stages utilize the full residual of the governing equation, thereby formally eliminating the splitting error altogether. Likewise, Lu et al. [30] consider an alternative balanced/re-balanced splitting strategy originally proposed by Speth et al. [29] and derive a midpoint integration rule that also effectively eliminates the splitting error.

In the present work, we adapt the above operator splitting strategies to develop schemes for handling stiff chemistry within the dual-time framework. We propose two new schemes, both of which incorporate an external, stiff ODE solver for the chemistry integration. The main attraction of such an approach is that it potentially allows using the same scheme for pseudo-time integration, including the local time-stepping and low-Mach preconditioning algorithms that have been optimized for non-reacting flows. The proposed operator-splitting schemes also avoid the drawbacks of the fully-coupled approach such as reduced iterative efficiency and the need for *ad hoc* corrections to the scheme.

The first scheme is a natural extension of the Strang splitting scheme applied in physical time. In this case, the dual-time

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