



A dynamic adaptive method for hybrid integration of stiff chemistry



Yang Gao^a, Yufeng Liu^a, Zhuyin Ren^b, Tianfeng Lu^{a,*}

^a Department of Mechanical Engineering, University of Connecticut, Storrs, CT 06269-3139, United States

^b Center for Combustion Energy and School of Aerospace Engineering, Tsinghua University, Beijing 100084, China

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ABSTRACT

The operator-splitting schemes for integration of stiff diffusion–reaction systems were found to fail in error control, i.e. incurring $O(1)$ relative errors, with splitting time steps larger than that required for fully explicit integration, when significant non-chemical radical sources are present. It was shown that, by excluding the transport term from the chemistry integration, errors by orders of magnitude may occur in radical concentrations solved in the chemistry sub-step, resulting in significant errors in the major species. The failing scenario is demonstrated with a toy problem and an unsteady perfectly-stirred reactor (PSR) for hydrogen/air with significant H radical concentration at inlet. A dynamic adaptive method for hybrid integration (AHI) of stiff chemistry is then proposed as a substitute for the operator-splitting schemes in such cases. The AHI method can obtain accurate solutions by integrating the fast species and reactions implicitly and the non-stiff terms, including slow reactions and non-chemical source terms, explicitly. Specifically, fast species and reactions are identified on-the-fly based on their analytically derived timescales, the rates of slow variables are evaluated explicitly and those of fast species are evaluated partial-implicitly. As such, the number of variables to be implicitly solved at each integration time step is reduced to the number of the fast species, resulting in a smaller Jacobian matrix and consequently lower computational cost compared with the fully implicit solvers. The hybrid method is validated in auto-ignition for hydrogen/air with different equivalence ratios and initial temperatures, and compared with the Strang splitting scheme for the toy problem and the unsteady PSR. Results show significant improvement in accuracy using the AHI method.

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1. Introduction

Detailed chemistry is important for high-fidelity reacting flow simulations. Major challenges to incorporate detailed chemistry in large-scale simulations are primarily attributed to the large sizes and severe stiffness of detailed chemistry. While detailed mechanisms can be reduced in size through skeletal reduction and timescale analyses [1], chemical stiffness renders the low-cost explicit integration solvers inapplicable for many flow simulations, particularly when relatively large time steps are adopted, and computationally expensive implicit solvers are typically required to integrate combustion problems. Chemical stiffness is induced by the extremely short timescales associated with highly reactive radicals and fast reactions. In direct numerical simulations (DNS) of compressible reacting flows, the time steps are typically limited by the fine spatial resolution and the Courant–Friedrichs–Lewy (CFL) condition, such that the typical step sizes for time-integration

are smaller than, say, 10 ns [2], and in such cases chemical stiffness can be removed on-the-fly without significant overhead due to the sparse coupling of the fast chemical processes [3]. However, stiffness removal for simulations with significantly larger integration time steps remains a challenge due to the densely-coupled fast chemical processes, particularly the fast reactions that are in partial equilibria. While such timescale analyses as computational singular perturbation (CSP) [4,5] and intrinsic low dimensional manifold (ILDM) [6] can be employed to systematically eliminate the short timescales of fast modes, significant computational overhead is involved with the methods based on Eigen-analysis such that the overall computational time is comparable to or even higher than that using the implicit solvers, e.g. VODE [7] and DASAC [8], which are widely adopted in practical reacting flow simulations.

The computational overhead of implicit solvers is primarily attributed to the Jacobian evaluation and LU decomposition. As such, the computational cost is typically $O(n^2)$, where n is the number of species, for small to moderately large mechanisms where the Jacobian evaluation is through numerical perturbations and dominates the computational cost, and $O(n^3)$ for large mechanisms

* Corresponding author.

E-mail address: tlu@engr.uconn.edu (T. Lu).

where the LU decomposition is the most time consuming operation. Evaluation of the Jacobian matrix can typically be expedited through analytic techniques [1], and the high computational cost associated with LU decomposition can be reduced by preconditioning [9] and sparse matrix techniques [10–13], and linear scaling with large mechanisms for spatially homogenous reactor calculations was observed.

For simulations of multi-dimensional flows, fully implicit integration schemes typically induce high computational costs due to the large number of spatial grid points involved. Implicit–Explicit (IMEX) approaches combine implicit and explicit discretizations for different source terms for reduced computational cost [14–18]. Operator-splitting schemes [19–26] are frequently used to integrate stiff chemistry and non-chemical processes in separate sub-steps, such that the expensive implicit solvers are only invoked for the integration of local chemistry, while the low cost explicit solvers can be employed to integrate the non-chemical source terms. In particular, the Strang splitting scheme [26] is among the most widely used operator splitting schemes for practical combustion simulations. It features second-order accuracy for sufficiently small splitting time steps and is rather straightforward to implement. While error control of the splitting schemes has been well studied at the limit of small splitting time steps, the splitting time steps adopted in most practical simulations are typically moderately large to avoid excessively high computational cost, and such cases with moderately large splitting time steps are referred to as coarse cases [22]. Splitting errors induced by stiff chemistry in coarse cases can be rather large [27], although successes have been reported in many studies, e.g. [21,25,28]. The mechanisms for the large splitting errors in coarse cases can be complex and are not fully understood.

In the present study, a mechanism associated with stiff chemistry that can result in failed error control of operator-splitting schemes in coarse cases is identified. The reason of the failure is attributed to the significant modification of the slow chemistry's trajectory by operator splitting, i.e. by excluding the transport source term from the sub-step for chemistry integration. A dynamic adaptive method for hybrid integration (AHI) is then proposed as a substitute of the operator-splitting schemes to integrate combustion systems involving stiff chemistry with improved accuracy.

As the outline of this paper, the large splitting errors of the Strang splitting scheme in coarse cases are first demonstrated and investigated using a toy problem. An AHI method is then proposed to resolve this issue and to achieve accurate and efficient time-integration of stiff chemistry coupled with transport. The AHI method is tested in auto-ignition and the solutions are compared with that from SENKIN [29], which utilizes the fully implicit DASAC solver based on the backward difference formula (BDF). The results of AHI are then compared with that of the Strang splitting scheme for the toy problem and an unsteady perfectly stirred reactor (PSR) of hydrogen/air using detailed chemistry.

2. The Strang splitting scheme and a toy problem

The Strang splitting scheme is among the most widely used solvers for reacting flows involving stiff chemistry, for which the spatially discretized governing equations can be expressed as:

$$\frac{d\Phi}{dt} = \mathbf{M}(\Phi) + \mathbf{S}(\Phi) \quad (1)$$

where Φ is the vector of the thermo-chemical composition, including, e.g. temperature and species mass fractions. The operators \mathbf{M} and \mathbf{S} are for the transport and chemistry terms, respectively. To solve Eq. (1) using the second-order Strang splitting scheme

[25,26], the time domain $[t_0, t_f]$ is discretized into n_t uniform intervals of size Δt , which are referred to as the splitting time steps. In each splitting time step, time-integration can be performed in the following sequence, namely the $\mathbf{S}/2 - \mathbf{M} - \mathbf{S}/2$ scheme:

$$\frac{d\Phi^{(1)}}{dt} = \mathbf{S}(\Phi^{(1)}), \quad \Phi^{(1)}(0) = \Phi^n \quad \text{on } [0, \Delta t/2] \quad (2a)$$

$$\frac{d\Phi^{(2)}}{dt} = \mathbf{M}(\Phi^{(2)}), \quad \Phi^{(2)}(0) = \Phi^{(1)}(\Delta t/2) \quad \text{on } [0, \Delta t] \quad (2b)$$

$$\frac{d\Phi^{(3)}}{dt} = \mathbf{S}(\Phi^{(3)}), \quad \Phi^{(3)}(0) = \Phi^{(2)}(\Delta t) \quad \text{on } [0, \Delta t/2] \quad (2c)$$

where Φ^n is the composition at the beginning of the n th splitting time step. The initial conditions of Eqs. (2b) and (2c) are the solutions of Eqs. (2a) and (2b), respectively, and $\Phi^{(3)}(\Delta t/2)$ is the solution at the end of the splitting time step. Eq. (2b) can typically be explicitly integrated in one step if the splitting time step is sufficiently small to resolve the transport term, while Eqs. (2a) and (2c) typically require multiple implicit steps using stiff ODE solvers. Note that one can build a $\mathbf{M}/2 - \mathbf{S} - \mathbf{M}/2$ scheme in a similar manner, which is nevertheless less accurate than the $\mathbf{S}/2 - \mathbf{M} - \mathbf{S}/2$ scheme as discussed in [22]. The $\mathbf{S}/2 - \mathbf{M} - \mathbf{S}/2$ scheme will be used to study the splitting errors in the following.

A toy model is first constructed to investigate the possible scenarios where the operator splitting schemes may fail in coarse cases. The model involves the following three reactions.



where k_1 , k_2 and k_3 are the reaction rate coefficients of reactions R_1 , R_2 , R_3 , respectively. Species A is the reactant, B is the product, C is an intermediate species that is not of direct importance to A and B , and R is a radical that controls the important reaction (R_3) for product formation. The parameter α determines the overall reaction order and nonlinearity of (R_3).

For simplicity, the transport term of species R is set to be a constant, d , and those for the other species are set to be zero. The term d mimics the effect of a mixture, e.g. in the preheat zone of a premixed flame, receiving substantial amount of radicals from a neighboring fluid element, e.g. in the reaction zone. Note that including nontrivial transport terms for the major species does not affect the nature of the toy problem.

The dependent variables and source terms in Eq. (1) for the toy problem can thereby be expressed as:

$$\begin{aligned} \Phi &= [A, B, C, R]^T, \\ \mathbf{S} &= [-k_1 A - k_3 A R^\alpha, k_3 A R^\alpha, k_2 R, k_1 A - k_2 R]^T, \\ \mathbf{M} &= [0, 0, 0, d]^T, \end{aligned} \quad (3)$$

with the initial condition being

$$A = 1, B = C = R = 0, \quad \text{at } t = 0$$

k_2 is chosen to be much larger than k_1 , i.e. $k_2 \gg k_1$, such that R stays in quasi steady state (QSS) after an initial transient period and can be approximated as

$$R \approx \frac{k_1 A + d}{k_2} \quad (4)$$

and the timescale of R can be defined as $\tau = 1/k_2$. It is seen that the concentration of R is sensitive to transport unless $|d| \ll k_1 A$.

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