

Operator-Splitting in Reacting Flow Modeling

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Abstract

We present two numerical formulations utilizing operator-splitting in the context of multi-dimensional reacting flow. In both cases, symmetric Strang-type splitting is utilized to ensure second-order time accuracy. The first case involves splitting the reaction and diffusion terms in a finite difference formulation for the propagation of a reacting scalar field. This is done to allow the use of specialized efficient integration procedures for each of the diffusion and reaction terms. The second case involves the splitting of Eulerian and Lagrangian components in a coupled Lagrangian-Eulerian reacting flow implementation where new Lagrangian elements are created inside the computational domain by a source term on the Eulerian mesh. We demonstrate second-order accuracy in both cases, and discuss the role of various parameters in determining accuracy and efficiency.

Introduction

Operator splitting [1] is desirable in many numerical time integration applications for reducing computational effort. On the other hand, it can affect time-integration accuracy due to “splitting” errors related to the decoupling of inherently coupled physical processes. Thus, care is necessary to maintain adequate accuracy when operator splitting is implemented.

We will discuss the utilization of operator splitting in the context of two different time integration schemes as applied to chemically reacting flow. The first pertains to reaction-diffusion coupling in a flame, while the second pertains to the convective-diffusive-baroclinic coupling of vorticity and scalar fields in a hybrid Eulerian-Lagrangian reacting flow model. In each case, splitting was used to decouple two or more physical processes, leading to enhanced computational efficiency. For each scheme, we describe the utility of splitting, present the requisite algorithm construction for second-order time accuracy, and the error behavior.

Reaction-Diffusion Coupling

Flames are largely determined by underlying reaction-diffusion balances, and are therefore useful testbeds for operator splitting. Due to the large ranges of spatial and temporal scales involved, explicit time integration of reacting flow equations has typically two bottlenecks: the stiffness of the chemical source terms, and the diffusional stability restriction. Both lead to the need for small time steps, rendering detailed multidimensional flame computations very expensive. At the outset, we choose not to use fully implicit schemes because the associated memory requirements with detailed kinetics are severe. Further, accuracy considerations suggest that the time step size must be kept smaller than the smallest physically relevant time scale in the flow, and the convective CFL number should be maintained less than unity, rendering a fully implicit implementation counter-productive.

The goal is then to integrate diffusion and chemical source terms efficiently, accurately, and with reasonable memory overhead, in the context of explicit convection. Such a scheme is presented below, using a second-order operator-split implicit-explicit (IMEX) construction for decoupling the diffusion from the stiff integration [2, 3] of the reaction source terms. The scheme is constructed by splitting each global time step symmetrically into two diffusion half-steps interspersed by a reaction step. The convection term is split uniformly among the three steps. Each diffusion half step is integrated using $M/2$ fractional steps of size $\Delta t' = \Delta t/M$. This allows the utilization of a large global time step Δt , while the diffusional stability constraint is satisfied by $\Delta t'$. The reaction step is integrated using a stiff ODE integration procedure (DVODE [4]).

To illustrate, consider a scalar equation : $\partial\phi/\partial t = C + D + R$, with C , D , and R denoting convective, diffusive, and reactive terms. Let M be the number of diffusive sub-steps of size $\Delta t' = \Delta t/M$. Define $S_C^n = \frac{3}{2}C^n - \frac{1}{2}C^{n-1}$ as the second-order Adams-Bashforth (AB2) formulation for C at t^n , and S_D as a similar formulation for D . S_D is based on a second-order Runge Kutta (RK2) discretization in the first fractional step of each diffusion half-step, and on AB2 for subsequent sub-steps. The following operator-split integration of this equation from t^n to $t^{n+1} = t^n + \Delta t$, with $\phi^n \rightarrow \phi^{n+1}$, is second order in Δt :

1. $\hat{\phi}^k - \hat{\phi}^{k-1} = \Delta t' \left(S_C^n/2 + \hat{S}_D^{k-1} \right)$, for $k = 1, 2, \dots M/2$; $\hat{\phi}^0 = \phi^n$.
2. $\tilde{\phi}^{M/2} - \hat{\phi}^{M/2} = \Delta t S_C^n/2 + \int_{\Delta t} R(\phi) dt$
3. $\tilde{\phi}^k - \tilde{\phi}^{k-1} = \Delta t' \left(S_C^n/2 + \tilde{S}_D^{k-1} \right)$, for $k = \frac{M}{2} + 1, \frac{M}{2} + 2, \dots M$; $\phi^{n+1} = \tilde{\phi}^M$.

where the integral in step 2 denotes the implicit stiff integration procedure.

The above scalar conservation equation is implemented as one component of a full low-Mach-number reacting flow model. In general a system of such equations is implemented for species and energy conservation in addition to the momentum, continuity, and state equations [2, 3]. We integrate the momentum equations using a projection method [5], with a fractional time-step procedure, similar to that in the above diffusional half-steps, implemented for the viscous terms. The overall time-accuracy of the scheme is expected to be a function of the global time step Δt , the number of scalar and momentum fractional steps, and the absolute and relative error tolerances implemented in the stiff-integrator.

Lagrangian-Eulerian Coupling

Lagrangian vortex methods [6], where the vorticity field is discretized using circulation-carrying Lagrangian vortex elements, have been used successfully for efficient modeling of flow dynamics in both non-reacting and reacting flow. However, the application of these techniques to flames has been limited to using constant properties and unity Lewis numbers. On the other hand, Eulerian methods, e.g. finite differences, can easily deal with detailed transport and chemical kinetics. Thus, the utility of a hybrid construction that uses a finite-difference scheme for scalar transport and the vortex method for the momentum equations is self-evident. We have developed an adaptive mesh refinement finite difference implementation for efficient discretization of multidimensional flames. This was coupled with a vortex method implementation that uses fast multipole N -body velocity evaluations [7]. The construction utilizes discrete expansion sources to handle the expansion field due to combustion heat release, and provides for the generation of baroclinic vorticity. In the present context, we focus on the vorticity coupling issues between the two schemes as regards time integration errors and their convergence rate. The governing equations are tightly coupled. Scalar fields are propagated on the mesh using velocities evaluated from the vortex elements, and both baroclinic vorticity generation due to local scalar gradients, and vorticity diffusion, lead to the production of new Lagrangian elements with requisite circulation. Note that, whereas a second-order non-split diffusive update of existing particle strengths (no particle injection) is possible [8], and is routinely used in the context of the Particle Strength Exchange (PSE) scheme for vorticity diffusion, we have found the application of such a non-split procedure with particle injection to be first order in time. Moreover, while the extension of PSE to the present case, whereby mesh-generated circulation is added to existing particles, would be preferred, we have not found a consistent and accurate means to achieve this. On the other hand, the following symmetric split construction with particle injection is conservative and does yield second-order time accuracy.

Consider a simplified model problem that includes (1) a set of vortex elements at locations $\chi = \{\chi_p\}$, with circulations $\Gamma = \{\Gamma_p\}$, describing a 2D patch of vorticity, (2) a scalar field ϕ defined on a mesh that overlays the domain, and (3) a circulation source term S evaluated on the mesh as a function of the velocity ($\mathbf{v}$) and the scalar field (ϕ). The governing equations may be written as:

$$\frac{\partial\phi}{\partial t} = R(\phi, \mathbf{v}), \quad \frac{d\chi}{dt} = \mathbf{v}(\chi, \Gamma), \quad \frac{d\Gamma}{dt} = S(\mathbf{v}, \phi)$$

where,

$$\phi(\mathbf{x}, 0) = \phi^0, \quad \chi(0) = \delta\chi^0, \quad \Gamma(0) = \delta\Gamma^0.$$

The circulation source term is used to create new vortex elements $(\delta\chi, \delta\Gamma)$ at mesh cell centers at each time step. Thus, the set of vortex elements at $t^n = n\Delta t$ is:

$$\begin{bmatrix} \chi^n \\ \Gamma^n \end{bmatrix} = \bigcup_{k=0}^n \begin{bmatrix} \delta\chi^k \\ \delta\Gamma^k \end{bmatrix}.$$

The present scheme involves two RK2 updates of (ϕ, χ) , each over $\Delta t' = \Delta t/2$, interspersed by injection of new elements and RK2-update of their strengths over Δt , as follows:

1. RK2 scalar and vortex element location update over $\Delta t'$,

$$\begin{bmatrix} \hat{\phi} \\ \hat{\chi} \end{bmatrix} = \begin{bmatrix} \phi^n \\ \chi^n \end{bmatrix} + \frac{1}{2} \begin{bmatrix} R^n + R(\tilde{\phi}, \tilde{\mathbf{v}}) \\ \mathbf{v}^n + \tilde{\mathbf{v}} \end{bmatrix} \Delta t', \quad \text{where} \quad \begin{bmatrix} \tilde{\phi} \\ \tilde{\mathbf{v}} \end{bmatrix} = \begin{bmatrix} \phi^n + R^n \Delta t' \\ \mathbf{v}(\chi^n + \mathbf{v}^n \Delta t', \Gamma^n) \end{bmatrix}$$

2. Create new zero-strength vortex elements at mesh cell centers $(\bigcup_{ij} \mathbf{x}_{ij})$ and update their strengths with RK2 over Δt ,

$$\begin{aligned} \hat{\chi}^* &= \hat{\chi} \cup \delta\chi^*, & \delta\chi^* &= \bigcup_{i,j} \mathbf{x}_{ij}, & \hat{\Gamma}^* &= \Gamma^n \cup \delta\Gamma^* \\ \delta\Gamma^* &= \hat{S}\Delta t, & \hat{S} &= S(\hat{\mathbf{v}}, \hat{\phi})|_{\delta\chi^*}, & \hat{\mathbf{v}} &= \mathbf{v}(\hat{\chi}, \Gamma^n) \\ \Gamma^{n+1} &= \Gamma^n \cup \delta\Gamma^n, & \delta\Gamma^n &= \frac{1}{2}(\hat{S} + S(\mathbf{v}^*, \hat{\phi})|_{\delta\chi^*})\Delta t, & \mathbf{v}^* &= \mathbf{v}(\hat{\chi}^*, \hat{\Gamma}^*) \end{aligned}$$

where $S()|_{\delta\chi^*}$ indicates that S is evaluated at the locations $\delta\chi^*$. This results in a set of vortex elements at locations $\hat{\chi}^*$ with strengths Γ^{n+1} .

3. RK2 scalar and vortex element location update over $\Delta t'$,

$$\begin{bmatrix} \phi^{n+1} \\ \chi^{n+1} \end{bmatrix} = \begin{bmatrix} \hat{\phi} \\ \hat{\chi}^* \end{bmatrix} + \frac{1}{2} \begin{bmatrix} R(\hat{\phi}, \hat{\mathbf{v}}^*) + R(\tilde{\phi}^*, \tilde{\mathbf{v}}^*) \\ \hat{\mathbf{v}}^* + \tilde{\mathbf{v}}^* \end{bmatrix} \Delta t', \quad \begin{bmatrix} \tilde{\phi}^* \\ \tilde{\mathbf{v}}^* \end{bmatrix} = \begin{bmatrix} \hat{\phi} + R(\hat{\phi}, \hat{\mathbf{v}}^*)\Delta t' \\ \mathbf{v}(\hat{\chi}^* + \hat{\mathbf{v}}^* \Delta t', \Gamma^{n+1}) \end{bmatrix}$$

where $\hat{\mathbf{v}}^* = \mathbf{v}(\hat{\chi}^*, \Gamma^{n+1})$.

Discussion

The above two constructions deal with different numerical problems, yet they share similarities through their use of Strang splitting [1], involving application of a subset of the governing operators to two half-time-step integration steps separated by a full-time-step application of the remaining operator(s). The behavior of resulting time-integration errors, and their coupling to other errors (e.g. spatial discretization errors), is specific to each case. The reaction-diffusion problem, which requires a specification of the implicit stiff-integration convergence thresholds, exhibits coupling between the explicit and implicit time integration errors. This plays a role in the optimal choice of the number of diffusion sub-steps M , and the efficiency of the scheme. Similarly, implementation of the Eulerian-Lagrangian procedure necessitates periodic redistribution of vortex elements to reduce their number, such that the final time-accuracy of the scheme depends on the redistribution frequency, and the associated interpolation kernel. Nevertheless, using numerical convergence studies with Δt -refinement, we find the inherent time integration errors for both schemes to be second order, as illustrated in Figures 1 and 2. This is remarkable given the various additional components of each scheme, namely stiff integration, multi-step and predictor-corrector constructions, particle injection, and particle-mesh coupling.

The talk will provide, in light of recent computational results, a detailed discussion of error behavior and the role of numerical parameters.

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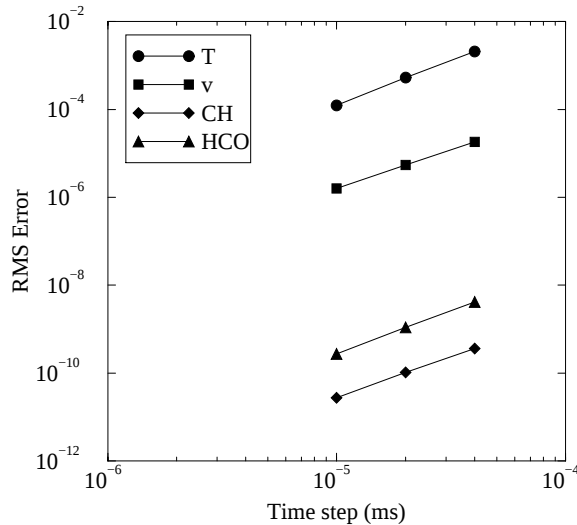


Figure 1. RMS error convergence results for a 1D flame using the operator-split stiff scheme. The results are based on $M = 16$ fractional steps for scalar diffusion and four for momentum diffusion. The RMS error is between solutions with successive global time-step refinement, at a fixed time instant. The figure illustrates the second-order decay of the error in temperature T , velocity v , and CH and HCO mole fractions with the global time step Δt .

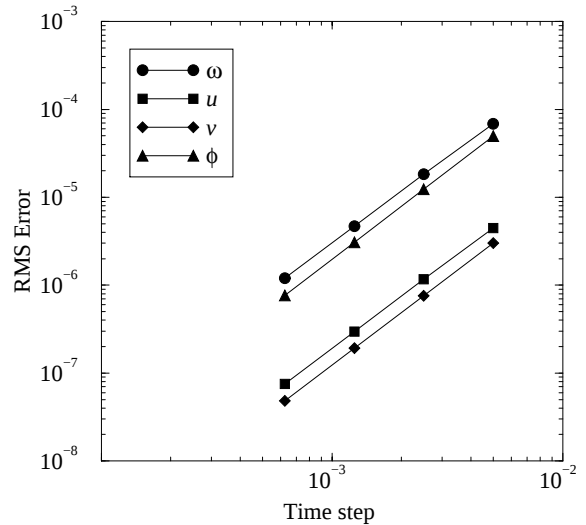


Figure 2. RMS error convergence results for a 2D decaying gaussian vortex and scalar distributions, using the coupled Lagrangian-Eulerian scheme. The scalar and vorticity fields are transported by convection and diffusion. A circulation source term $S(\mathbf{v}, \phi)$ is utilized involving second derivatives of the vorticity field and first derivatives of the scalar field. The RMS error is between solutions with successive global time-step refinement, at a fixed time instant. The figure illustrates the second-order decay of the error in vorticity ω , the velocity (u, v), and the scalar ϕ with the global time step Δt .