

# High-Order Operator-Splitting Methods for Reacting Gas Dynamics

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Mathematical models that describe the dynamics of reacting flows consist of systems of partial differential equations (PDEs), which specify the advection, diffusion, and reaction of chemical species within a moving medium and which couple the effects of non-reactive hydrodynamics with the effects of heat release in the chemical reactions. The characteristic time scales of the chemical reactions are much shorter than the hydrodynamic time scales, which are determined by the local sound speed, and the diffusive time scales. Nonlinear forcings may introduce spatial variations that appear in the solutions as sharp reaction fronts or shocks. Thus, the construction of numerical methods that accurately and efficiently handle the widely-differing time scales and sharp gradients is of significant interest.

In the absence of diffusion and reaction, the model equations become Euler equations, the hyperbolic nature of which requires the use of specialized techniques. Many well-established numerical methods for hyperbolic equations exist, e.g., ENO (essentially non-oscillatory), Godunov, PPM (piecewise parabolic method), and TVD (total-variation-diminishing) methods, etc. Most of these methods are based on conservative flux difference discretization, solution of Riemann problems, and application of limiters, which together ensure correction propagation of shocks and avoid oscillations or smearing. These methods may be incorporated into multiscale numerical methods for reacting gas dynamics.

Because of the disparity in time scales, the equations for the reactive gas dynamics model become stiff, with the reaction terms much stiffer than the advection and diffusion terms. The method of lines (MOL) is a common approach to the numerical integration of advection-diffusion-reaction (A-D-R) equations, of which the model reactive Navier-Stokes equations are a special case. The MOL first discretizes the equations in space, resulting in

a large coupled system of ordinary differential equations (ODEs), which are then integrated in time. To avoid prohibitively small time steps imposed by the stiffness of the reaction and diffusion terms in the ODEs, these terms must be integrated implicitly.

When applied to the system of ODEs obtained via a MOL discretization, fully implicit methods treat every term implicitly and require the solution of implicit fully coupled equations. In contrast, semi-implicit methods handle the advection term explicitly and integrate the diffusion and reaction terms implicitly. Because the reaction terms are typically nonlinear and the diffusion terms are typically non-local, the solution of such implicit equations can be computationally expensive, especially when the number of chemical species is large. Moreover, because the same (small) time step, the size of which is restricted by the stiffness of the reactions, is used for all processes, the computational cost of a fully implicit or semi-implicit method can be significant.

Alternatively, an operator-splitting or time-splitting approach may be used. In an operator-splitting approach, processes are decoupled and integrated sequentially, resulting in implicit equations that are easier to solve. Moreover, by integrating slower processes using larger time steps, the overall computational cost can be reduced. As noted previously, the advection step of a conservative method usually involves the solution of a Riemann problem, which can be computationally expensive; thus, the computational time may be substantially reduced by using a larger advection time step. However, in addition to the numerical errors arising in the integration of each term, the operator-splitting approach also introduces splitting errors, which reduce the accuracy of the approximation.

In a previous study [1], high-order multi-implicit spectral deferred correction (MISDC) methods are presented for the solution of A-D-R equations. MISDC methods are similar to operator-splitting methods in that these methods give rise to multiple implicit equations, for which different time steps may be used. By eliminating both the integration and splitting errors, MISDC methods can in theory generate solutions with arbitrarily high temporal accuracy. MISDC methods are a generalization of spectral deferred correction methods [2], which use a low-order numerical method to compute a high-order approximation. This is achieved by using the low-order numerical method to solve a series of correction equations, each of which increases the order of accuracy of the approximation. Numerical results in [1] suggest that for problems with stiff diffusion and reaction terms, MISDC methods

can be constructed which compare favorably with semi-implicit Runge-Kutta methods.

Because temporal integration is the main focus in [1], spatial discretization is done using sixth-order centered differencing, which assumes that the solution is smooth. However, as noted previously, solutions in models of reactive gas dynamics may have sharp gradients, which cannot be accurately resolved by centered differencing. Thus in this study, PPM is incorporated within MISDC methods for problems involving sharp fronts. The resulting methods—the conservative MISDC methods—compute approximations to the cell-averaged or finite-volume solution of the model equations via a MOL discretization on the flux difference form of the equations. Numerical results show that the conservative nature of the methods allows a robust representation of discontinuities and sharp gradients and demonstrate the expected convergence rates for the methods of orders three, four, and five.

## References

- [1] A. Bourlioux, A. T. Layton, and M. L. Minion. High-order multi-implicit spectral deferred correction methods for problems of reactive flow. Submitted to *J. Comput. Phys.* 2002.
- [2] A. Dutt, L. Greengard, and V. Rokhlin. Spectral deferred correction methods for ordinary differential equations. *BIT*, 40 (2): 241–266, 2000.