

A semi-Lagrangian Discontinuous Galerkin method for efficient atmospheric chemistry modelling

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The development of accurate and conservative numerical methods to solve efficiently the linear advection equation

$$(0.1) \quad \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c) = 0$$

has always been a main goal of the research on advection dominated flows. In this context, the semi-Lagrangian (SL) method is widely acknowledged as an accurate and efficient option. In SL methods, equation (0.1) is reformulated in Lagrangian form

$$(0.2) \quad \frac{dc}{dt} = \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = -c \operatorname{div} \mathbf{u}$$

and time discretization exploits the fact that the solution values are available along the characteristic lines, which are approximated numerically. The original formulation of SL methods, however, is inherently non conservative, so that, in order to achieve local mass conservation, two main approaches are typically pursued.

In the first strategy, based on conservative remapping, equation (0.2) is formally integrated over a control volume that is *moving with the flow*, and then discretized by approximate reconstruction of the upstream control volume. In the second strategy, more similar in spirit to Eulerian finite volume methods, equation (0.1) is first integrated in space over a *fixed mesh control volume*. It is then integrated in time over a time step Δt , and finally it is discretized by approximate reconstruction of the flux through the control volume boundary over Δt . The resulting methods can be referred to as flux form SL schemes.

The purpose of the present work is to introduce a flux form SL discretization for (0.1) that employs a Discontinuous Galerkin (DG) formulation to reconstruct the numerical solution within each control volume. Throughout the paper, the novel technique is referred to as semi - Lagrangian Discontinuous Galerkin (SLDG) approach. The properties of the proposed method are analyzed here assuming the advective flow \mathbf{u} in (0.1) to be incompressible. Furthermore, a simple monotone approach based on the Flux Corrected Transport algorithm has also been introduced, which was shown to lead to discrete solutions satisfying the maximum principle while greatly reducing the loss of accuracy at the extrema usually associated with this technique. Finally, one possible approach to

include diffusive terms in the mathematical model is also discussed in the present work, although a full understanding of the optimal way to treat diffusion in conjunction with SLDG requires further study.

The SLDG method aims at combining the accuracy and conservation property of the DG method with the computational efficiency and robustness of SL techniques. On one hand, the use of SL backward trajectories allows to achieve unconditional stability, irrespective of the value of the Courant number, thus overcoming the severe stability restrictions enforced by the DG formulation. On the other hand, the potential loss of accuracy of standard SL methods at low Courant numbers does not affect the SLDG scheme, as demonstrated by a number of numerical experiments. Furthermore, in the case of large systems of advection–diffusion–reaction equations, as typical of environmental modelling applications, the extra effort needed to compute the trajectories is required only once for the whole system, so that the potential overhead associated with this effort becomes negligible. Finally, the proposed method is characterized by a computational stencil that is similar to those of standard Eulerian DG formulation. This means that high–order approximations can be constructed locally, without involving a large number of neighbouring elements, thus making domain decomposition–based parallelization approaches more straightforward. The use of an elementwise variable–degree formulation is also possible, leaving unaltered the global and local mass conservation properties of the scheme. As an example of the results that can be obtained with the proposed method, tracer advection of a discontinuous profile has been computed with SLDG and with the more standard Runge Kutta, Eulerian time discretization associated to $P1$ discontinuous finite elements. It can be seen that more accurate results can be achieved in spite of a much larger time step.

	Rel. L^2 error	Rel. L^∞ error	Dissipation error	Dispersion error	Cons. error
SLDG	2.26e-01	1.49e+00	1.02e-03	4.30e-02	-2.75e-15
RKDG	3.61e-01	1.59e+00	1.06e-02	1.01e-01	1.30e-15
	$\min(c_h)$	$\max(c_h)$	$\min(c_{h,0})$	$\max(c_{h,0})$	
SLDG	-1 - 4.76e-01	1 + 5.41e-01	-1 - 1.33e-10	1 + 1.00e-13	
RKDG	-1 - 7.09e-02	1 + 9.74e-02	-1 - 2.22e-16	1 + 2.22e-16	

Table 0.1: Errors for the SLDG solution ($C = 2$) and RKDG solution ($C = 0.3$) in the Doswell deformation flow test case.

The SLDG method is currently being implemented in the framework of the Lokal-Modell nonhydrostatic atmospheric model, in order to perform numerical prediction of pollutant transport and atmospheric chemistry phenomena over the Italian peninsula. The accuracy and efficiency advantages listed above are expected to reduce significantly the cost of such computationally intensive simulations.

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