A Runge Kutta Discontinuous Galerkin approach to solve reactive flows on structured and unstructured grids: the parabolic and source operators.

Juliette Ryan*, Germain Billet* and Michel Borrel*
Corresponding author: billet@onera.fr

* ONERA, France.

Abstract: A Runge-Kutta Discontinuous Galerkin method ($RKDG$) to solve the parabolic and source parts of reactive Navier-Stokes equations written in conservation form is presented. The parabolic operator uses two different recovery methods. The physical model involves complex chemistry and detailed transport. Test cases in structured and unstructured meshes are presented.

Keywords: Numerical Algorithms, Discontinuous Galerkin, Computational Fluid Dynamics, Reactive flows, Navier-Stokes equations.

1 Introduction

In [1], we described a Runge-Kutta Discontinuous Galerkin ($RKDG$) method that solves the hyperbolic part of the reactive NS equations written in conservation form. Herein, we focus our attention on the parabolic and source terms of the reactive NS equations. The transport fluxes are expressed in terms of transport coefficients and macroscopic variable gradients. The transport coefficients are functions of the state of the mixture, i.e., of pressure, temperature and species mass fractions. The molar production rates are of Maxwellian type and are compatible with the law of mass action.

Nowadays, there are two categories of methods to solve the parabolic terms. In the first one, the scheme is devised through a mixed formulation by introducing an equation for the gradient that takes into account the jump of the solution at interfaces. The scheme needs to be stabilized by either interior penalty (IP) terms or numerical viscosity terms with parameters to be adjusted. Depending on the formulation, the resulting scheme is either compact or non compact. Among the main contributors, we can cite Bassi and Rebay with their BR1 and BR2 methods, Baumann and Oden, Cockburn and Shu with the LDG method, Peraire and Persson with the CDG method, Liu and Yan with the DDG method, Brezzi and al. with the symmetric IP method. Gassner and al. show the link between their diffusive generalized Riemann solver and the IP approach.

A second category is based on local reconstruction or recovery of the solution to smooth the discontinuities. van Leer [2]-[3] was the first to propose the so-called Recovery method where the viscous fluxes at element boundaries are computed by merging the adjacent elements and defining on this new element a locally smooth P_{2k+1} recovered solution that is in the weak sense indistinguishable from the piecewise discontinuous P_k solution. This method eliminates

the artificial introduction of penalty terms and the tuning of parameters. This approach is very accurate and efficient on structured grids [4] but an impediment is the construction of the local merging basis and the need to solve a linear problem at each interface which can be awkward if we use an adaptive strategy on unstructured grids. On unstructured grids, a simpler numerical procedure is chosen (EDG method) [5]. This method is a sequel to the shift cell technique that uses the Green formula that reconstructs the gradient by projection on the shift cell basis. For 2-D simulations, the jumps across element boundaries are eliminated in the computation of the viscous fluxes using a projection of the piecewise P_k discontinuous solution on the P_k basis of the overlapping rectangular elements. In this paper, we use both approaches, van Leer recovery method on the structured meshes and the EDG method on the unstructured meshes.

Because of the great number of equations, the expressions of the transport coefficients and the chemical reactions, it appears judicious to limit the method order to DGP^2 with the reactive flows in order to have realistic computational costs. In all the simulations, a third-order TVD Runge-Kutta RK^3 scheme is associated with a DGP^2 approach. 1-D test cases with RK^3DGP^2 are compared with a 6^{th} order finite difference code. The first case is the 1-D propagation of a complex acoustic waves produced by a viscous gaseous interface. The second case is a 1-D sinusoidal reactive mixing of mass and temperature. And last, 2-D simulations are proposed on structured and unstructured grids. The first one concerns the diffusion of a circular thermal and density interface. The second test case presents a draughtboard reactive mixing $H_2 - O_2$ within a varying temperature field, first in a flow at rest (low Mach number flow). Then, the fields are distorted by a strong unsteady shear flow (subsonic and supersonic flows) (see Fig. 1).

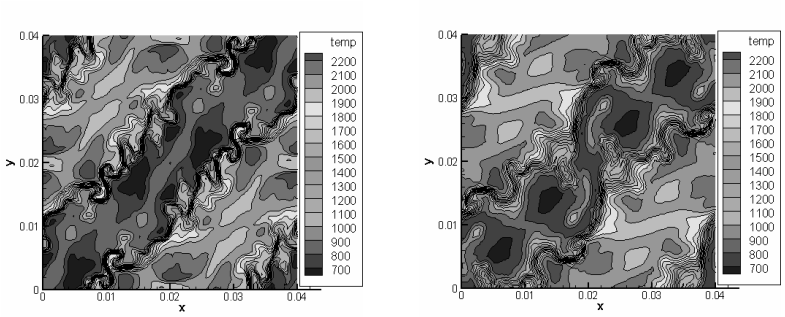

Figure 1: Temperature field at $t = 6.\ 10^{-4}s$ with a subsonic flow (left: Cartesian grid results with 10000 elements; right: triangular grid results with 8256 elements).

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