[5-D-01] Direct Discontinuous Galerkin Methods for the Reacting, Multi-Species, 3D Compressible Navier-Stokes Equations

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Direct Discontinuous Galerkin Methods for the Reacting, Multi-Species, 3D Compressible **Navier-Stokes** Equations

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Abstract: The Direct Discontinuous Galerkin (DDG[1]) method and a counterpart with Interface Correction (DDGIC[2]) are extended to compute viscous terms that arise when solving the compressible Navier-Stokes equations in thermo-chemical nonequilibrium. The DG formulation is solved on 3D unstructured grids. Thermodynamic properties, transport properties, chemical reaction rates, and energy exchange terms are computed using Mutation++[3]. A method for determining the homogeneity tensor of the flow equations required for DDGIC is shown. A number of numerical experiments are conducted to assess the accuracy and performance of the method. The numerical results indicate that DDG and DDGIC provide accurate solutions and perform well for general flows in thermo-chemical nonequilibrium.

1 Introduction

Discontinuous Galerkin (DG) methods are a subset of finite element methods which have garnered significant interest in CFD applications for their accuracy, flexibility, and robustness in advection dominated problems. The discretization of elliptical terms, however, becomes a complex issue due to derivatives being multivalued at element interfaces. Taking the simple average of the derivatives at the interface on either side is unstable. There are many methods to solve this problem, such as: interior penalty methods, local discontinuous Galerkin, and the methods of Bassi and Rebay; these are all described in detail by Arnold et al [4]. In 2009, Liu and Yan published the direct discontinuous Galerkin (DDG) method [1]; unlike previous approaches, this method doesn't require recasting the second order derivatives as a system of first order derivatives. This makes code design and flux computation much simpler. DDG, however, doesn't achieve (k + 1) order of convergence for k-order polynomials when k is an even number; to combat this, Liu and Yan [5] introduced an interface correction, which has been extended to the 2D Navier-Stokes equations by Danis and Yan [2]. In this work, the original DDG method and the DDG with Interface Correction (DDGIC) method of Danis and Yan is extended to three dimensions and reacting flows in thermo-chemical non-equilibrium.

Vector Symbols:

$oldsymbol{U}$	vector of conservative quantities
\boldsymbol{F}_{i}^{v}	fluxes due to viscous effects
Physical Quantities	
ρ_s	density of species s
E	total specific energy
p	pressure
T	temperature
q_j	heat flux in direction j
$\dot{\omega}_s$	mass rate of production of species s
D_s	diffusion coefficient for species s
κ	heat conductivity
x_j	the spatial Cartesian coordinate
Y_s	species mass fraction $\frac{\rho_s}{\rho}$
$e_{V,s}$	vibrational energy of species s
$\dot{\Omega}_s^V$	vibrational energy production and relaxation for species s
ns	number of species

- convective fluxes
- $oldsymbol{F}_{j}^{c} oldsymbol{S}$ chemical source terms
- mixture density $\left(\sum_{s} \rho_{s}\right)$ ρ
- internal specific energy e E_V
- vibrational specific energy velocity component in direction x_i
- u_i T_V vibrational temperature
- shear stress tensor τ_{ij}
- enthalpy of species s h_s
- vibrational heat flux q_{Vi}
- species diffusion flux for species s J_{sj}
- mixture dynamic viscosity μ
- vibrational heat conductivity κ_V
- ttime
- energy production
- Ω_s for species s

2 Problem Statement

2.1 Governing Equations

Consider the 3D, compressible, reacting, multispecies, Navier-Stokes equations:

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{F}_{j}^{c}(\boldsymbol{U})}{\partial x_{j}} = \frac{\partial \boldsymbol{F}_{j}^{v}(\boldsymbol{U}, \nabla \boldsymbol{U})}{\partial x_{j}} + \boldsymbol{S}(\boldsymbol{U})$$
(1)

Where:

$$\boldsymbol{U} = \begin{pmatrix} \rho_{1} \\ \vdots \\ \rho_{ns} \\ \rho u_{i} \\ \rho E \\ \rho E_{V} \end{pmatrix}, \quad \boldsymbol{F}_{j}^{c} = \begin{pmatrix} \rho_{1} u_{j} \\ \vdots \\ \rho_{ns} u_{j} \\ \rho u_{i} u_{j} + p \delta_{ij} \\ u_{j} (\rho E + p) \\ u_{k} \rho E_{V} \end{pmatrix}, \quad \boldsymbol{F}_{j}^{v} = \begin{pmatrix} -J_{1,j} \\ \vdots \\ -J_{ns,j} \\ \tau_{ij} \\ u_{i} \tau_{ij} + q_{j} - \sum_{s} h_{s} J_{s,j} \\ q_{Vj} - \sum_{s} e_{V,s} J_{s,j} \end{pmatrix}, \quad \boldsymbol{S} = \begin{pmatrix} \dot{\omega}_{1} \\ \vdots \\ \dot{\omega}_{ns} \\ 0 \\ 0 \\ \dot{\Omega}_{V}^{V} \end{pmatrix}$$
(2)

The total density ρ is defined such that:

$$\rho = \sum_{s=1}^{ns} \rho_s \tag{3}$$

The shear stress tensor and heat flux vectors are computed by:

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3} \mu \frac{\partial u_l}{\partial u_l} \delta_{ij}, \quad q_j = -\kappa \frac{\partial T}{\partial x_j} - \kappa_V \frac{\partial T_V}{\partial x_j}, \quad q_{vj} = -\kappa_V \frac{\partial T_V}{\partial x_j} \tag{4}$$

The equation of state is closed using the ideal gas law:

$$p = \rho RT \tag{5}$$

The total specific energy (E) is related to the internal specific energy (e) by the addition of kinetic energy

$$E = e + \frac{1}{2} \sum_{j} u_j u_j \tag{6}$$

The species diffusion fluxes are computed using a modified form of Fick's Law to conserve mass [6]:

$$J_{s,j} = \rho \Big(-D_s \frac{\partial Y_s}{\partial x_j} + Y_s \sum_{l=1}^{ns} D_l \frac{\partial Y_l}{\partial x_j} \Big)$$
(7)

The thermodynamic properties (such as species enthalpies h_s), transport properties (including viscosity μ , thermal conductivities κ and κ_V , and average diffusion coefficients D_s), chemical source terms ($\dot{\omega}_s$), and energy exchange term ($\dot{\Omega}_V$) are computed using Mutation++ [3].

3 Numerical Methods

Introduce the broken Sobolev space over the equation domain $\Omega \subset \mathbb{R}^3$

$$V^{s,p}(\Omega) = \{ v \in L^p(\Omega) : \forall |\alpha| \le s, D^{\alpha}v \in L^p(\Omega) \}$$
(8)

Let \mathcal{T}_h represent a triangulation of Ω with non-overlapping elements \mathcal{K} . Let $\Gamma = \partial \mathcal{K}$ represent the element interfaces and n_j represent the *j*th component of the outward unit normal vector. Then define

the semi-discrete weak form of the governing equations over the elements \mathcal{K} :

$$\frac{\partial}{\partial t} \int_{\mathcal{K}} \boldsymbol{U} v \, d\mathcal{K} - \int_{\mathcal{K}} \boldsymbol{F}_{j}^{c}(\boldsymbol{U}) \frac{\partial v}{\partial x_{j}} \, d\mathcal{K} + \int_{\Gamma} \hat{\boldsymbol{F}}_{j}^{c}(\boldsymbol{U}) v n_{j} \, d\Gamma = \\ - \int_{\mathcal{K}} \boldsymbol{F}_{j}^{v}(\boldsymbol{U}, \nabla \boldsymbol{U}) \frac{\partial v}{\partial x_{j}} \, d\mathcal{K} + \int_{\Gamma} \hat{\boldsymbol{F}}_{j}^{v}(\boldsymbol{U}, \nabla \boldsymbol{U}) v n_{j} \, d\Gamma + \int_{\mathcal{K}} \boldsymbol{S} v \, d\mathcal{K} \quad \forall v \in V^{s, p}(\Omega) \quad (9)$$

The interface convective flux \hat{F}_{j}^{c} is calculated using HLLC [7] or LDFSS [8] while the interface viscous flux \hat{F}_{j}^{v} is calculated using one of the two DDG methods.

3.1 Original DDG

The original DDG flux prescribes a method for determining the gradients of quantities at the interface from the corresponding left and right values, gradients, and second derivatives. Consider a quantity ϕ that has two states at a disontinuous cell interface (ϕ^+ and ϕ^- respectively) as well as the respective gradients and second derivatives. Define the jump and average operators as follows:

$$[\![\phi]\!] = \phi^+ - \phi^-, \quad \overline{\phi} = \frac{\phi^+ + \phi^-}{2} \tag{10}$$

Then the DDG gradient of the quantity is:

$$\frac{\overline{\partial \phi}}{\partial x_j} = \beta_0 \frac{\llbracket \phi \rrbracket}{\Delta} n_j + \frac{\overline{\partial \phi}}{\partial x_j} + \beta_1 \Delta \llbracket \frac{\partial^2 \phi}{\partial x_i \partial x_j} \rrbracket n_i$$
(11)

Where β_i are coefficients as prescribed by Liu and Yan [1]; this is dependent on the polynomial order of the approximation. In this work, for DG(P1), the value $\beta_0 = 1.7$ is used. For *k*th order polynomials, Danis and Yan [2] choose $\beta_0 = k^2$ for the heat equation and $\beta_0 = (k+1)^2$ for the Navier-Stokes equations. Note: for even polynomial orders this will not achieve (k + 1) order of convergence. It is possible to recover the (k + 1) convergence order by using *k*th order derivatives of the solution and corresponding coefficients as outlined by Liu and Yan [5]. However, this is better remedied by the interface correction. The characteristic distance Δ is calculated at each quadrature point using a dimension agnostic strategy outlined by Cheng et al. [9] using the centroids of the left and right element domains c^- and c^+ respectively, the quadrature point coordinates q_{Γ} , and the unit normal vector \boldsymbol{n} . This is illustrated in Figure 1.

$$\Delta = |q_{\Gamma} - c^{-}| \cdot \boldsymbol{n} + |q_{\Gamma} - c^{+}| \cdot \boldsymbol{n}$$
(12)



Figure 1: Calculation of Characteristic width Δ

The DDG gradients can be evaluated component-wise for vector quantities to obtain a vector of gradients that is single valued at the interface.

$$\widehat{\nabla U} = \frac{\widehat{\partial U}}{\partial x_j} = \beta_0 \frac{\llbracket U \rrbracket}{\Delta} n_j + \frac{\overline{\partial U}}{\partial x_j} + \beta_1 \Delta \Bigl[\Bigl[\frac{\partial^2 U}{\partial x_i \partial x_j} \Bigr] n_i$$
(13)

Then the numerical flux is computed using the DDG derivatives and the average quantities at the

interface as:

$$\widehat{\boldsymbol{F}}_{j}^{v} = \boldsymbol{F}_{j}^{v}(\overline{\boldsymbol{U}}, \widehat{\boldsymbol{\nabla}\boldsymbol{U}}) \tag{14}$$

3.2 DDGIC

Danis and Yan [2] define DDGIC for nonlinear homogeneous fluxes. This means that the flux can be written in the form:

$$\boldsymbol{F}_{i}(\boldsymbol{U},\nabla\boldsymbol{U}) = \mathbf{G}(\boldsymbol{U})\nabla\boldsymbol{U} \tag{15}$$

In addition, the diffusion tensor \mathbf{G} is assumed to be positive definite. For clarity, this will sometimes be written in index notation:

$$F_{ik}(\boldsymbol{U},\nabla\boldsymbol{U}) = G_{ikrs}(\boldsymbol{U})\frac{\partial U_r}{\partial x_s}$$
(16)

3.2.1 Computation of Diffusion Tensor

Klaij, Van der Vegt, and Van der Ven [7] provide an explicit version of the diffusion tensor for the singlespecies compresesible Navier-Stokes equations. The diffusion tensor can be calculated by differentiation by considering the property of homogeneous functions:

$$\frac{\partial F(U, \nabla U)}{\partial (\nabla U)} = \mathbf{G}(U) \tag{17}$$

However, for more complex functions, it can be simpler and easier to verify by breaking the flux F into components that are linear combinations of U multiplied by the gradients U. The matrix of conservative variable derivatives can be written as:

$$\frac{\partial U_r}{\partial x_s} = \begin{bmatrix} \frac{\partial \rho_l}{\partial x_s} & & \frac{\partial u_j}{\partial x_s} & & \frac{\partial \rho E}{\partial x_s} & & \frac{\partial \rho E_V}{\partial x_s} \end{bmatrix}^T \quad l \in 1, ..., ns \quad j \in 1, ..., d$$
(18)

Where ns is the number of species and d is the number of spatial dimensions. It now becomes straightforward to write quantities that arise in the diffusion matrices in the same form as above, knowing that the tensors will be contracted with the conservative variable gradients along the r and s indices. The species mass fraction derivatives tensor can be written as:

$$\left(\frac{\partial Y_l}{\partial x_k}\right)_{rs} = \frac{1}{\rho} \begin{bmatrix} \delta_{sk} \delta_{rl} - \delta_{sk} Y_l & 0 & 0 \end{bmatrix}^T$$
(19)

Visualizing the contraction with which conservative variable gradients in Equation 18 can be accomplished by envisioning overlaying these terms on Equation 18.

As an implementation note, the Kronecker deltas can be treated as holding those indices equal and only looping over one of the two indices. An implementation of the species mass fraction derivatives tensor:

```
1 \quad dYmat(:, :, :, :) = 0.0
_{2} do l = 1, ns
       do k = 1, d
3
            s = k !kroneker
4
            do r = 1, ns
\mathbf{5}
                dYmat(s, r, k, l) = -Y(l) / rho
6
            end do
7
            r = 1
8
            dYmat(s, r, k, 1) = dYmat(s, r, k, 1) + 1.0 / rho
9
        enddo
10
11
   enddo
```

The species diffusion matrix for Fick's Law can be expressed as a linear combination of the mass

fraction derivatives tensor and conservative variables:

$$\left(J_{i,k}\right)_{rs} = -\rho D_i \left(\frac{\partial Y_i}{\partial x_k}\right)_{rs} + \rho Y_i \sum_l D_l \left(\frac{\partial Y_l}{\partial x_k}\right)_{rs} \tag{20}$$

Let $r_u = r - ns$ represent the indices corresponding to the $\frac{\partial u_j}{\partial x_s}$ terms in Equation 18 – where ns is the number of species. The velocity gradient tensor is:

$$\left(\frac{\partial u_i}{\partial x_k}\right)_{rs} = \frac{1}{\rho} \begin{bmatrix} -\delta_{ks} u_i & \delta_{ks} \delta_{r_u i} & 0 \end{bmatrix}^T \quad i \in 1, ..., d$$

$$\tag{21}$$

The original quantity is recovered by tensor contraction of the r and s indices:

$$\left(\frac{\partial u_i}{\partial x_k}\right)_{rs} \frac{\partial U_r}{\partial x_s} = \frac{\partial u_i}{\partial x_k} \tag{22}$$

The shear stress term in its entirety can be written as:

$$\left(\tau_{ij}\right)_{rs} = \frac{\mu}{\rho} \left[-\delta_{js}u_s - \delta_{is}u_s + \frac{2}{3}\delta_{ij}u_s \quad \left| \quad \delta_{js}\delta_{r_ui} + \delta_{is}\delta_{r_uj} - \frac{2}{3}\delta_{ij}\delta_{r_us} \quad \left| \quad 0 \quad \left| \quad 0 \right]^T$$
(23)

For the temperature derivatives, Gnoffo et al [10] provide equations based on the conservative variable gradients

$$\frac{\partial T}{\partial x_j} = -\frac{\frac{\partial e}{\partial x_j} - \frac{\partial E_V}{\partial x_j} - \sum_s \frac{\partial Y_s}{\partial x_j} (e_s - E_{V,s})}{C_{v,TR}}$$
(24)

$$\frac{\partial T_V}{\partial x_j} = \frac{\frac{\partial E_V}{\partial x_j} - \sum_s \frac{\partial Y_s}{\partial x_j} E_{V,s}}{C_{v,V}}$$
(25)

Where $C_{v,TR}$ and $C_{v,V}$ are the specific heats for translational-rotational energy modes, and vibrational energy modes respectively and are obtained from the conservative variables through Mutation++ [3]. The derivatives of e and E_V are computed as follows:

$$\frac{\partial e}{\partial x_j} = \frac{1}{\rho} \left(\frac{\partial \rho E}{\partial x_j} - E \frac{\partial \rho}{\partial x_j} - u_l \frac{\partial \rho u_l}{\partial x_j} + ||u|| \frac{\partial \rho}{\partial x_j} \right)$$
(26)

$$\frac{\partial E_V}{\partial x_j} = \frac{1}{\rho} \left(\frac{\partial \rho E_V}{\partial x_j} - E_V \frac{\partial \rho}{\partial x_j} \right)$$
(27)

Where $||u|| = \sum_{l} u_{l}u_{l}$ is the velocity magnitude. Let i_{e} and $i_{E_{v}}$ represent the indices for the energy and vibrational energy terms. The tensors for the energy derivatives are then:

$$\left(\frac{\partial e}{\partial x_k}\right)_{rs} = \frac{1}{\rho} \begin{bmatrix} \|u\| - E & | & -\delta_{r_u i} u_i & | & \delta_{i_e r} & | & 0 \end{bmatrix}$$
(28)

$$\left(\frac{\partial E_V}{\partial x_k}\right)_{rs} = \frac{1}{\rho} \begin{bmatrix} E_V & | & 0 & | & \delta_{i_{E_V}r} \end{bmatrix}$$
(29)

(30)

From this the tensors for the temperature derivatives are:

$$\left(\frac{\partial T}{\partial x_j}\right)_{rs} = \frac{1}{C_{v,TR}} \left(\left(\frac{\partial e}{\partial x_j}\right)_{rs} - \left(\frac{\partial E_V}{\partial x_j}\right)_{rs} - \sum_{l=1}^{ns} \left(\frac{\partial Y_l}{\partial x_j}\right)_{rs} (e_l - E_{V,l}) \right)$$
(31)

$$\left(\frac{\partial T_V}{\partial x_j}\right)_{rs} = \frac{1}{C_{v,V}} \left(\left(\frac{\partial E_V}{\partial x_j}\right)_{rs} - \sum_{l=1}^{ns} \left(\frac{\partial Y_l}{\partial x_j}\right)_{rs} E_{V,l} \right)$$
(32)

where e_l and $E_{V,l}$ are the species energies and vibrational energies respectively, which are computed by

Mutation++. Finally the viscous flux tensor can be assembled by:

$$G_{ikrs}(\boldsymbol{U}) = \begin{pmatrix} -\left(J_{1k}\right)_{rs} & & \\ \vdots & & \\ -\left(J_{(ns)k}\right)_{rs} & & \\ \left(\tau_{jk}\right)_{rs} & & \\ u_{j}\left(\tau_{jk}\right)_{rs} - \kappa\left(\frac{\partial T}{\partial x_{k}}\right)_{rs} - \kappa_{V}\left(\frac{\partial T_{V}}{\partial x_{k}}\right)_{rs} - \sum_{l} h_{l}\left(J_{lk}\right)_{rs} \\ -\kappa_{V}\left(\frac{\partial T_{V}}{\partial x_{k}}\right)_{rs} & \end{pmatrix}$$
(33)

3.2.2 Computation of the Viscous Fluxes and Interface Correction

The DDGIC flux uses the diffusion matrix evaluated at the average state at the interface. Recall the definition of the diffusion matrix:

$$F_{ik}^{v}(\boldsymbol{U},\nabla\boldsymbol{U}) = G_{ikrs}(\boldsymbol{U})\frac{\partial U_{r}}{\partial x_{s}}$$
(34)

Then applying substituting the averages and gradients results in:

$$\widehat{F}_{ik}^{v}(\boldsymbol{U},\nabla\boldsymbol{U}) = G_{ikrs}(\overline{\boldsymbol{U}})\frac{\widehat{\partial U_r}}{\partial x_s}$$
(35)

The interface correction is an additional term which utilizes the direction vector $\boldsymbol{\xi}$. This direction vector is the interface unit normal transformed by the diffusion tensor:

$$\xi_{irs} = G_{ikrs} n_k \tag{36}$$

Rewriting the semi-discrete weak form with the DDGIC flux and interface correction terms:

$$\frac{d}{dt} \int_{\mathcal{K}} \mathbf{U}v \, d\mathcal{K} - \int_{\mathcal{K}} \mathbf{F}_{j}^{c}(\mathbf{U}) \frac{\partial v}{\partial x_{j}} \, d\mathcal{K} + \int_{\Gamma} \hat{\mathbf{F}}_{j}^{c}(\mathbf{U}) v n_{j} \, d\Gamma = -\int_{\mathcal{K}} \mathbf{F}_{j}^{v}(\mathbf{U}, \nabla \mathbf{U}) \frac{\partial v}{\partial x_{j}} \, d\mathcal{K}
+ \int_{\Gamma} \xi_{irs}(\mathbf{U}) \frac{\partial U_{r}}{\partial x_{s}} v \, d\Gamma - \frac{1}{2} \int_{\Gamma} \llbracket U_{r} \rrbracket \xi_{irs}(\mathbf{U}) \frac{\partial v}{\partial x_{s}} \, d\Gamma + \int_{\mathcal{K}} \mathbf{S}v \, d\mathcal{K} \quad \forall v \in V^{s,p}(\Omega) \quad (37)$$

4 Numerical Results

Some canonical test cases are run to compare the effectiveness of different DDG formulations with a 2nd Order Finite Volume scheme. All formulations of the DDG schemes compute fluxes for the conservative quantities as described above. In computing the DDG gradients as in Equation 13, two different choices of variable sets are investigated for the original DDG method to compute the $\llbracket U \rrbracket$ and $\frac{\partial U}{\partial x_j}$ terms. The first will be noted by (VT):

$$\boldsymbol{U}^{(VT)} = \begin{bmatrix} \rho_1 \\ \vdots \\ \rho_{ns} \\ u_i \\ T \\ T_V \end{bmatrix}$$
(38)

The second is the standard conservative variable set as described in Equation 2. The LDFSS inviscid flux is used for high speed flows.

4.1 Multispecies Flatplate

An inert 2-species air mixture ($Y_{O_2} = 0.233$, $Y_{N_2} = 0.767$) is blown at Mach 0.2 over a flat plate with an adiabatic wall boundary condition. This case is run with a single temperature; i.e., the vibrational energy terms are omitted. The skin friction and y-velocity profile are compared with the analytic Blasius solution. The y-velocity shows the benefits of using the DDG over a second-order finite volume scheme. There is little conclusive difference between the different DDG implementations.



Figure 2: Density Contour at Front of Plate



(b) y-velocity profile at x = 0.99L

Figure 3: Comparison of DDG(P1) and finite volume for flow over a flat plate

4.2 High Enlthalpy Hypersonic Cylinder

This case is modeled after Nastac et al. [11] section IV.B. High enthalpy hypersonic ($M_{\infty} \approx 8.7$) flow around a cylinder is studied. The cylinder radius is 45 mm and the length is 380 mm. The 5 species

model for air from Park et al. (1985) [12] is used for the species definition and reaction mechanisms. Thermodynamic and transport properties are evaluated using Mutation++. A rigid-rotor harmonic oscillator model is used for thermodynamics. Transport properties are based on collision integrals, with the mixture-averaged viscosity computed using the Gupta-Yos approximation and thermal conductivity using Wilke's mixing rule.

$$\begin{split} Y_{O_2} &= 0.134 \\ Y_O &= 0.0795 \\ Y_{NO} &= 0.0509 \\ Y_N &= 0.0 \\ Y_{N_2} &= 0.7356 \\ M_\infty &= 8.76 \\ P_\infty &= 697.038 \text{ Pa} \\ T_\infty &= 694 \text{ K} \\ T_{V,\infty} &= 694 \text{ K} \end{split}$$

The cylinder walls are an isothermal boundary condition at 300 K. The mesh used is an unadapted hexahedral mesh with one cell in the z-direction. Results are compared with results from NASA's DPLR code[13] to serve as a qualitative benchmark in Figure 5. A mesh comparison is shown in Figure 6. The DDG results are in good agreement with the computational results from DPLR. There are some differences in shock standoff distance, maximum temperature, and maximum pressure – given that the two codes use different discretizations and thermochemistry implementations, small differences in the code comparison are to be expected.

The heat fluxes on the surface of the cylinder show that all the DDG schemes give good quantitative results which closely match the experiment by Karl et al. [14].



Figure 4: Cylinder surface heat flux comparison





Figure 5: Results Comparison of DDG(P1) - (PV gradients) (Left) and DPLR (Right)



Figure 6: Center Slice of Hexahedral mesh used (Left), 2D DPLR unadapted mesh for qualitative comparison (Right)

Pressure, temperatures, mach number, and composition are compared along the stagnation line (from +y to the wall) in Figure 7. There are some inconsistencies along the stagnation line, likely due to differences in thermodynamics and transport properties. This work uses Mutation++ to compute thermophysical properties while DPLR uses its own internal databases and methods.



Figure 7: Stagnation Line Comparisons

4.3 High Enthalpy Hypersonic Flow Around a Hemisphere Cylinder

A primary goal of this work is to extend DDGIC to three dimensions. Therefore, we consider fully three-dimensional hypersonic flow over a hemisphere, based on the test case outlined in Section IV.D of Nastac et al. [11]. The same thermodynamics and chemical models are used as the previous case. Free

stream conditions are:

$$\begin{split} Y_{O_2} &= 0.134 \\ Y_O &= 0.0795 \\ Y_{NO} &= 0.0509 \\ Y_N &= 0.0 \\ Y_{N_2} &= 0.7356 \\ M_\infty &= 9.8 \\ P_\infty &= 697.038 \mbox{ Pa} \\ T_\infty &= 450 \mbox{ K} \\ T_{V,\infty} &= 450 \mbox{ K} \end{split}$$

The walls of the hemisphere cylinder are isothermal boundary conditions at 555.5 K. The mesh used is too coarse to fully resolve all the flow features so this primarily serves as a qualitative verification of 3D capabilities on a fully 3D geometry. The results in Figure 9 are reasonable when compared to the results in Nastac et al. [11] considering the differences in resolution. The low resolution mesh is used as a preliminary result for the available time and computing resources.



Figure 8: Mesh of central z-normal slice of the mesh



Figure 9: Mach number (top) and temperature (bottom) contours of the hemisphere cylinder on a central z-normal slice of the mesh

As a quantitative comparison, in Figure 10 we compare the surface heatfluxes with the experimental results obtained by Josyula and Shang[15] as referenced in Nastac et al. [11]. The heatfluxes follow the general contour of the experimental data, but for true agreement with the data higher resolution of the post-shock region is necessary.



Figure 10: Surface heat fluxes along a 45 degree cutplane with the *x*-coordinate normalized by the hemisphere radius.

5 Conclusions

Several implementations of DDG were extended to 3D flows with thermochemical non-equilibrium. Derivation and implementation are presented for the interface correction term extended to thermochemical nonequilibrium flows. Overall DDG is an effective scheme for flows in thermochemical equilibrium and recovered accurate skin friction in the flatplate benchmark case and accurate heat fluxes in the high enthalpy cylinder benchmark case.

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