**Министерство образования и науки Российской Федерации**

**Санкт-Петербургский политехнический университет Петра Великого**

**Национальное общество имитационного моделирования**

**Журнал "Компьютерные инструменты в образовании"**

**Группа компаний ТРАНЗАС**

**Европейская ассоциация EuroSim**

# КОМОД 2015

**Труды международной научно-технической конференции**

***1−3 июля 2015 года***

**Санкт-Петербург**
**Издательство Политехнического университета**
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# Using software package SIGMA for numerical simulation of nonequilibrium gas flows

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***Abstract*— A numerical method for solving of hypersonic nonequilibrium aerogasdynamics problems is suggested. The method is based on the full three-dimensional Navier-–Stokes equations, supplemented by the equations of chemical kinetics and the finite volume RKDG (Runge-Kutta Discontinuous Galerkin) method. The developed algorithms are implemented in the computer-aided software package SIGMA. The results of simulation of a hypersonic flow about a spherical nose segment of a model hypersonic vehicle are presented.**

***Keywords*— computational fluid dynamics, nonequilibrium aerogasdynamics, chemical kinetics, RKDG method, parallel processing.***

## I. Introduction (*Heading 1*)

When designing advanced hypersonic aircraft in many cases it is difficult to conduct experimental aerothermodynamics studies, and is impossible for flows with chemical reactions in air at high temperatures. Therefore, investigations of exterior problems of hypersonic aerodynamics considering multicomponent oncoming flow are based mainly on methods of mathematical and numerical simulation. However, there are difficulties that arise in numerical simulations associated with both the decomposition of a computational domain (meshing), and with the selection of a method for solving the system of partial differential equations that describe the behavior of the flow.

There are considerable number of works ([1]-[3], and others) devoted to numerical simulation of hypersonic gas flows taking into account these effects. Among the numerical methods the finite difference techniques based on TVD (total variation diminishing) schemes which have the necessary properties such as monotonicity of solutions and second-order approximation have gained widespread. However, it is very difficult to generate a smooth finite-difference grid when solving real problems with complex three-dimensional geometry of a body. Therefore, in such cases it is preferable to use unstructured grids with finite volume or finite element methods.

This paper studies the RKDG finite element method of second-order accurate and a compact template, which belongs to the class of TVD schemes, due to a separate procedure of monotonization. It saves the monotony of solutions and is applied for tetrahedral elements. Adaptation of this method for the integration of three-dimensional time-dependent partial differential equations over the tetrahedral grid was conducted. In addition to solving the gas dynamics equations, we considered the application of the RKDG method for the numerical integration of the equations for the concentrations of reactants of dissociated and ionized gas.

To generate a tetrahedral mesh is used finite difference adaptive mesh generator developed by the authors. In the generated regular mesh we allocated hexahedral elements, which are divided into tetrahedrons for applying the RKDG method. Generally each hexahedron is divided into five tetrahedrons and in some cases into six tetrahedrons. Such finite element meshes retain adaptation grid lines to geometry borders and allow to obtain solutions of better quality than with meshes generated by ordinary tetrahedral mesh generators. In addition the mesh generator allows to concentrate the grid lines in the direction of the body, which improves the accuracy of the calculation near the body.

We consider the Navier-Stokes equations with chemical kinetics, describing high-speed flow around an aircraft. Integration of the Navier-Stokes equations is performed by the splitting into physical processes. At the first stage the members of the viscous terms are excluded from the consideration. The problem is solved for ideal gas. Then the viscous term components are taken into account but do not take into account convection. Further the equations of chemical kinetics are solved in 3 stages. Firstly, an explicit-implicit scheme is used to solve the system of difference equations with source terms. Then the convection of the chemical components is taken into account. The system is solved by the RKDG method similarly the step of solving of inviscid flow. And then the diffusion of chemical components is taken into account. The algorithm for solving the equations is similarly the step of solving of viscous components.

The developed algorithms were implemented by the authors in their software package SIGMA [4]. SIGMA appropriates for simulation of supersonic and hypersonic flows, defining fields of mechanical and thermal stresses, as well as concentrations of chemical substances near the critical components of aerospace vehicles. SIGMA contains preprocessor, processor and postprocessor modules and is capable to perform calculations on high-performance computers. This approach is the further development of methods developed in the previous papers [5]-[6] by the authors.

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The results of a simulation of flow about a spherical nose segment of a model hypersonic aircraft are presented. The chemical gas-phase model included all the main components of high temperature air for flight conditions in the Earth's atmosphere. The peak wavelengths of the spectral intensity of the body have been obtained.

## THE SYSTEM OF EQUATIONS

Consider the system of equations of a viscous heat-conducting gas (the Navier-Stokes equations) with chemical kinetics:

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0, \\ \dfrac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + p\mathbf{E} - \mathbf{T}_v) = 0, \\ \dfrac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot ((\rho\varepsilon + p)\mathbf{v} - \mathbf{T}_v \cdot \mathbf{v} + \mathbf{q}) = 0, \\ \dfrac{\partial \rho y_i}{\partial t} + \nabla \cdot \rho y_i \mathbf{v} = \nabla \cdot (\rho D_{ij} \nabla \cdot y_i) + \omega_i \end{cases} \qquad (1)$$

where $\rho$ is the gas density of the gas mixture, $t$ is the time, $\mathbf{v}$ is the velocity vector of the center of mass of the mixture, $p$ is the pressure, $\mathbf{E}$ is the identity tensor, $\varepsilon$ is the total energy per unit volume, $y_i = \rho_i / \rho$ is the mass concentration of the *i*-th spice, $\omega_i$ is the source of generation of the *i*-th spice, $D_{ij}$ are the diffusion coefficients.

This system adds the relations for perfect gas, viscous stress tensor and heat flux vector:

$$p = \rho \frac{R_0}{M_0}\theta, \quad \frac{1}{M_0} = \sum_{i=1}^{7} \frac{y_i}{M_i}, \quad \varepsilon = e + \frac{|\mathbf{v}|^2}{2},$$

$$e = c_V \theta, \quad |\mathbf{v}|^2 = \mathbf{v}\cdot\mathbf{v}, \quad c_V = \sum_{i=1}^{7} y_i c_{Vi}, \quad \mathbf{q} = -\lambda \nabla \theta,$$

$$\mathbf{T}_v = -\frac{2}{3}\mu(\nabla \cdot \mathbf{v}) \cdot \mathbf{E} + \mu(\nabla \otimes \mathbf{v} + \nabla \otimes \mathbf{v}^T),$$

where $R$ is the universal gas constant, $M_i$ is the molecular weight of the *i*-th spice, $\theta$ is the gas temperature, $e$ is the internal energy per unit volume, $c_{Vi}$ is the specific heat at constant volume of the *i*-th spice, $\mu$ is the coefficient of viscosity, $\lambda$ is the thermal conductivity of the gas.

We consider the binary diffusion model. The coefficients of diffusion, viscosity and thermal conductivity are given by the following functions [7]:

$$D_{12} = 1.85 \cdot 10^{-7} \frac{\theta^{3/2}}{p \sigma_{12}^2 \Omega_{12}^{(1,1)}} \left( \frac{M_1 + M_2}{M_1 M_2} \right)^{1/2}, \quad \gamma_i = \frac{y_i}{M_i},$$

$$\mu = \sum_{i=1}^{6} \frac{\mu_i}{\left[ 1 + \sum\limits_{j=1, j\neq i}^{6} G_{ij}^{\mu} \dfrac{\gamma_j}{\gamma_i} \right]}, \quad \lambda = \sum_{i=1}^{6} \frac{\lambda_i}{\left[ 1 + \sum\limits_{j=1, j\neq i}^{6} G_{ij}^{\lambda} \dfrac{\gamma_j}{\gamma_i} \right]},$$

where $\sigma_{12}$ is the characteristic distance, $\Omega_{12}^{(1,1)}$ is the collision integral, $\mu_i$, $\lambda_i$ are the viscosity and thermal conductivity of pure gases, $G_{ij}^{\mu}$, $G_{ij}^{\lambda}$ are the universal constants.

The gas mixture consists of seven spices and the possible chemical reactions that occur in shock layer at high temperatures are following:

$$O_2 + M \rightleftarrows 2O + M, \quad N_2 + M \rightleftarrows 2N + M,$$
$$NO + M \rightleftarrows N + O + M, \quad NO + O \rightleftarrows O_2 + N,$$
$$N_2 + O \rightleftarrows NO + N, \quad NO + O \rightleftarrows NO^+ + e^-,$$

where $M$ is any of the six spices considered to be a catalyst, $e^-$ is the electronic component. Associate the index *i*=1,2,3,4,5,6 with the components of $O$, $N$, $NO$, $O_2$, $N_2$, $NO^+$ respectively.

Also the conditions of conservation of atomic composition

$$y_{O_2} = 0.21 - 0.5\left( y_O + y_{NO} + y_{NO+} \right),$$
$$y_5 = 0.79 - 0.5\left( y_N + y_{NO} + y_{NO+} \right),$$

and mixture quasineutrality $y_{NO+} = y_{e^-}$ are valid, thus only four spices are independent.

## II. NUMERICAL METHOD

The integration of the Navier-Stokes equations with chemical kinetics is performed by the method of the splitting into physical processes.

1. At the first stage the viscous and heat conduction terms are excluded from the consideration. The system of equations describing the ideal gas as follows

$$\mathbf{U}_t + \nabla \cdot \mathbf{F(U)} = \mathbf{0}, \qquad (2)$$

where $\mathbf{U} = [\rho, \rho v_x, \rho v_y, \rho v_z, \rho E]^{\mathrm{T}}$ is the vector of conservative variables, $\mathbf{F} = [\rho\mathbf{v}, \rho\mathbf{v} v_x + p\delta_1^i, \rho\mathbf{v} v_y + p\delta_2^i, \rho\mathbf{v} v_z + p\delta_3^i, \rho(E+p)\mathbf{v}]^{\mathrm{T}}$ is the flux function. For the solutions of the system of differential equations (1) are used RKDG method [8]. The system of basis functions $\varphi_i$, $i = \overline{1,4}$ is introduced, which have the following properties:

$$\varphi_i(x_i) = 1,\ \varphi_i(x_j) = 0,\ i \neq j,$$

where $x_i$ are the integration points of Second-Order Gaussian quadrature formulae for a tetrahedron [9]. The linear approximation of the vector $\mathbf{U}$ inside the tetrahedron is introduced $\mathbf{U}_h = \sum_{i=1}^{4} \varphi_i(x) \cdot u_i(t)$. Multiply the system (2) by the function $\varphi_i(x)$ and integrate over the tetrahedron. After simple transformations we obtain

$$\frac{V}{4}\frac{du_i(t)}{dt} = \int_V \mathbf{F}(\mathbf{U}_h)\nabla\varphi_i(x)\cdot dV - \\ - \int_S \tilde{\mathbf{F}}(\mathbf{U}_h^{int}, \mathbf{U}_h^{ext}) \cdot \varphi_i(x) \cdot dS, \quad (3)$$

where $V$ is the volume of the tetrahedron, $\tilde{\mathbf{F}}(\mathbf{U}_h^{int}, \mathbf{U}_h^{ext})$ is the numerical flux, which depends on the values of the vector of conservative variables into the tetrahedron $\mathbf{U}_h^{int}$ and the values inside the four neighboring tetrahedrons $\mathbf{U}_h^{ext}$. The numerical flux can be found, for example, by the HLLC method [10]. After this, the received system of ordinary differential equations (3) is solved by the Runge-Kutta method.

For proper simulation of shocks arising in hypersonic flows, it is necessary to carry out the procedure of monotonization for which TVD limiter is applied for each time step. Let us turn to the characteristic variable $\mathbf{V}$, multiplying the system (2) by the matrix of left eigenvectors of the matrix $\mathbf{A} = \frac{\partial \mathbf{F}}{\partial \mathbf{U}}$, $\mathbf{V} = \mathbf{L} \cdot \mathbf{U}$. A linear interpolation function for the tetrahedron can be written as: $\mathbf{V} = \mathbf{V}_m + (x - x_m)\boldsymbol{\alpha}_m + (y - y_m)\boldsymbol{\beta}_m + (z - z_m)\boldsymbol{\gamma}_m$, where index $m$ refers to the center of the tetrahedron, $\boldsymbol{\alpha}_m$, $\boldsymbol{\beta}_m$, $\boldsymbol{\gamma}_m$ are some coefficients. Next calculate the value of $\mathbf{V}_{\min} = \min\left(\mathbf{V}_m, \min_n \mathbf{V}_n\right)$ and $\mathbf{V}_{\max} = \max\left(\mathbf{V}_m, \max_n \mathbf{V}_n\right)$, where $\mathbf{V}_n$ are values at the centers of the adjacent tetrahedrons, $n = \overline{1,4}$. Min and max operation are applied to each element of the vector separately. Let us find the value of $\mathbf{V}_i$, $i = \overline{1,4}$ at the vertices of the tetrahedron. Then

$$\boldsymbol{\psi}_i = \begin{cases} \min\left(1, \dfrac{\mathbf{V}_{\max} - \mathbf{V}_m}{\mathbf{V}_i - \mathbf{V}_m}\right), & \text{if} \quad \mathbf{V}_i - \mathbf{V}_m > 0, \\ \min\left(1, \dfrac{\mathbf{V}_{\min} - \mathbf{V}_m}{\mathbf{V}_i - \mathbf{V}_m}\right), & \text{if} \quad \mathbf{V}_i - \mathbf{V}_m < 0, \\ 1, \quad \text{if} \quad \mathbf{V}_i - \mathbf{V}_m = 0. \end{cases}$$

Let $\boldsymbol{\psi} = \min(\boldsymbol{\psi}_1, \boldsymbol{\psi}_2, \boldsymbol{\psi}_3, \boldsymbol{\psi}_4)$, then the slope limiters $\boldsymbol{\psi}^T \cdot \boldsymbol{\alpha}_m, \boldsymbol{\psi}^T \cdot \boldsymbol{\beta}_m, \boldsymbol{\psi}^T \cdot \boldsymbol{\gamma}_m$ satisfy the TVD property. After applying the limiter we go back to the original conservative variables $\mathbf{U} = \mathbf{R} \cdot \mathbf{V}$, where $\mathbf{R}$ is the matrix of right eigenvectors of the matrix $\mathbf{A}$.

2. Then the viscous and heat conduction terms are taken into account but do not take into account convection. The system of equations look like:

$$\begin{cases} \mathbf{U}_t + \nabla \cdot \mathbf{T}(\mathbf{U}, \boldsymbol{\omega}) = 0, \\ \boldsymbol{\omega} = \nabla \cdot \boldsymbol{\Omega}, \end{cases} \quad (4)$$

where $\mathbf{T}(\mathbf{U}, \boldsymbol{\omega}) = [0, -\mathbf{T}_v, -\mathbf{T}_v \cdot \mathbf{v} + \mathbf{q}]$ and the matrix $\boldsymbol{\Omega}$ has the form:

$$\boldsymbol{\Omega} = \begin{bmatrix} v_x & 0 & 0 \\ 0 & v_y & 0 \\ 0 & 0 & v_z \\ v_y & v_x & 0 \\ v_z & 0 & v_x \\ 0 & v_z & v_y \end{bmatrix}.$$

The nabla operator is applied to the matrix row.

Same as the first stage we introduce the linear approximation inside the element:

$$\mathbf{U}_h = \sum_{i=1}^{4} \varphi_i(x) \cdot u_i(t), \qquad \boldsymbol{\omega}_h = \sum_{i=1}^{4} \varphi_i(x) \cdot \boldsymbol{\omega}_i(t).$$

Multiply the system (4) by the basis function $\varphi_i$, $i = \overline{1,4}$ we obtain:

$$\frac{V}{4}\frac{du_i(t)}{dt} = \int_V \mathbf{T}(\mathbf{U}_h, \boldsymbol{\omega})\nabla\varphi_i(x)\cdot dV - \int_S \tilde{\mathbf{T}}(\mathbf{U}_h^{int}, \boldsymbol{\omega}_h^{int}, \mathbf{U}_h^{ext}, \boldsymbol{\omega}_h^{ext}) \cdot \varphi_i(x) \cdot dS,$$

$$\boldsymbol{\omega}_i = \frac{4}{V}\left[\int_S \boldsymbol{\Omega} \cdot \mathbf{n}\varphi_i(x) \cdot dS - \int_V \tilde{\boldsymbol{\Omega}} \nabla\varphi_i(x) \cdot dV\right].$$

To find the numerical fluxes $\tilde{\mathbf{T}}$ and $\tilde{\boldsymbol{\Omega}}$ we use the central flux:

$$H(a,b)=\frac{1}{2}[H(a)+H(b)].$$

3. Further the equations of chemical kinetics are solved in 3 stages. Firstly, the mass fluxes of each *i*-th spice due to chemical transformation are taken into account:

$$\frac{\partial X_i}{\partial t}=\dot{\omega}_i, \qquad (5)$$

where $X_i=\frac{\rho y_i}{M_i}$ are molar concentration, $\dot{\omega}_i=\frac{\omega_i}{M_i}$. The source of generation of the *i*-th spice is calculated using the law of mass action:

$$\begin{aligned}
&\dot{\omega}_1=\varphi_{11}+\varphi_{13}+\varphi_{14}+\varphi_{15}+\varphi_{16},\\
&\dot{\omega}_2=\varphi_{22}+\varphi_{13}-\varphi_{14}-\varphi_{15}+\varphi_{16},\\
&\dot{\omega}_3=-\varphi_{13}+\varphi_{14}-\varphi_{15}, \quad \dot{\omega}_6=-\varphi_{16},\\
&\varphi_{11}=2k_1(K_1X_4-X_1^2),\\
&\varphi_{13}=k_3(K_3X_3-X_1X_2),\\
&\varphi_{14}=-k_4(K_4X_1X_3-X_2X_4),\\
&\varphi_{15}=-k_5(K_5X_1X_5-X_2X_3),\\
&\varphi_{16}=-k_6(K_6X_1X_2-X_6X_7),\\
&\varphi_{22}=2k_2(K_2X_5-X_2^2),
\end{aligned}$$

where $k_i$, $K_i$ are the specific rate of the reverse reactions and equilibrium constant, respectively, which are temperature-dependent [6].

The system (5) is solved by the explicit-implicit scheme [6]

$$\mathbf{X}^{n+1}=\tilde{\mathbf{X}}^{n+1}+\left[\mathbf{X}^n-\tilde{\mathbf{X}}^{n+1}+\Delta t\left(\alpha\dot{\boldsymbol{\omega}}^n+(1-\alpha)\tilde{\dot{\boldsymbol{\omega}}}^{n+1}\right)\right]\cdot \left[\mathbf{I}-(1-\alpha)\Delta t\left[\frac{\partial\tilde{\dot{\boldsymbol{\omega}}}^{n+1}}{\partial\mathbf{X}}\right]\right]^{-1}$$

where $\mathbf{X}=[X_1,X_2,X_3,X_6]^T$, $\tilde{\mathbf{X}}$ is the intermediate value of the iterative process, $\Delta t$ is time step, $\alpha$ is the blending coefficient (typically $\alpha=0.4$), $\mathbf{I}$ is the identity matrix.

4. Then the convection of chemical components is taken into account

$$\frac{\partial\rho y_i}{\partial t}+\nabla\cdot\rho y_i\mathbf{v}=0. \qquad (6)$$

The system (6) is solved by the RKDG scheme similarly the step of the solving of the inviscid flow.

5. And then the diffusion of chemical components is taken into account

$$\frac{\partial\rho y_i}{\partial t}=\nabla\cdot(\rho D_i\nabla\cdot y_i). \qquad (7)$$

The equations (7) are solved similarly the step of the solving of the viscous components.

## III. RESULTS

The simulation of the hypersonic flow about a spherical nose segment at Mach number $M$=20 and altitude $h$=30 km was considered. A solid ball had the following characteristics: radius $R$=30 cm, emissivity $\varepsilon$=1. The main goal of the simulation was the calculation of the spectral radiant intensity of the body as a function of wavelength.

Fig. 1-4 shows the three-dimensional distributions of gas-dynamic parameters near the body. The coating materials of the ball should be able to withstand extremely high temperature up to 6500$^o$K in the stagnation point. At such temperatures the processes of dissociation and ionization of air molecules occur. The initial concentrations of a mixture of molecular oxygen and nitrogen are changed and the new concentrations of atomic nitrogen and oxygen are generated near the body. The heat transfer coefficient, heat flux and spectral irradiances are calculated using the distribution of the temperature in the flow and on the surface of the blackbody. And it was obtained that the peak of wavelengths of the spectral intensity of the body is located in the near-infrared range.

## IV. CONCLUSIONS

A technique based on the RKDG method of the second order accurate for numerical solving of the full three-dimensional Navier--Stokes equations with chemical kinetics in domains of complicated forms, has been proposed. The formulation allows to take into account the changes in the chemical composition of the flow and calculates more accurately the integral characteristics of the gas mixture such as thermal conductivity, viscosity, specific heat, which effect on the mechanical and thermal stresses near the critical components of aerospace vehicles. The developed algorithms have been implemented in the computer-aided software package SIGMA. SIGMA appropriates for simulation of supersonic and hypersonic flows, defining fields of mechanical and thermal stresses, as well as concentrations of chemical substances near the critical components of aerospace vehicles. SIGMA contains preprocessor, processor and postprocessor modules and is capable to perform calculations on high-performance computers. The developed numerical method and software can be applied to the analysis of aerodynamics of hypersonic aircrafts.

The results of the simulation of the flow about the spherical nose segment of the model hypersonic aircraft are presented. The chemical gas-phase model included all the main components of high temperature air for flight conditions in the Earth's atmosphere. The peak wavelengths of the spectral intensity of the body have been obtained.

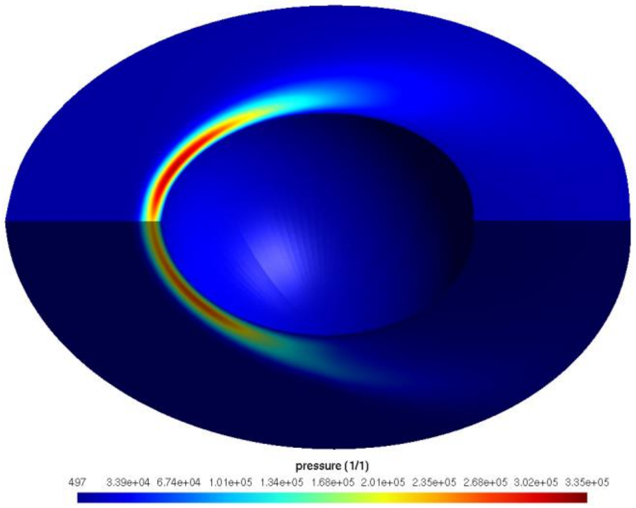


Fig. 1. Pressure *p*, Pa

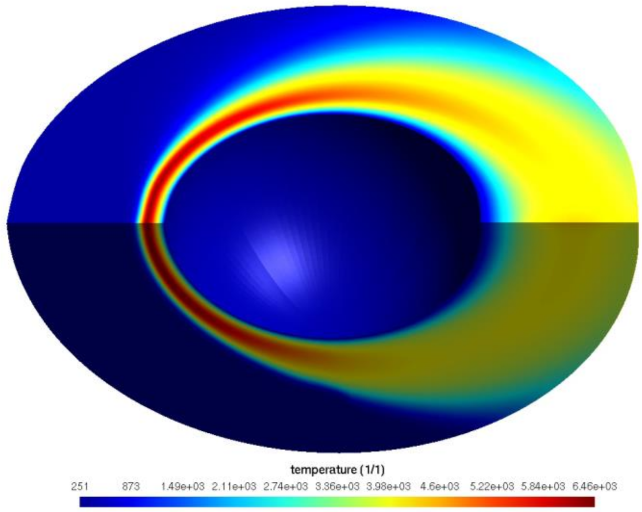


Fig. 2. Temperature θ, K

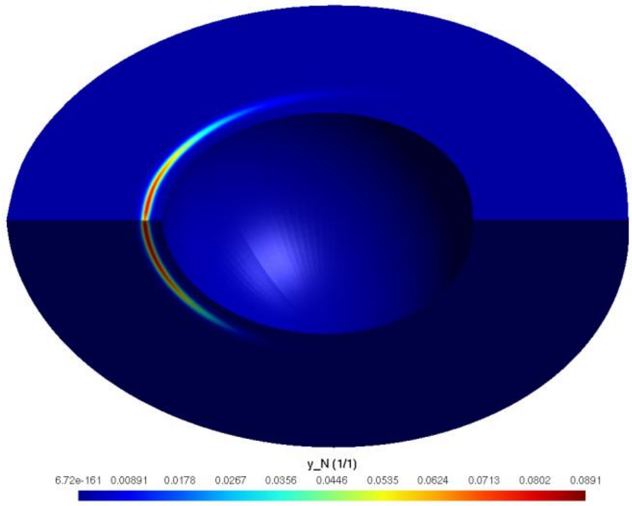


Fig. 3. Atomic nitrogen concentration

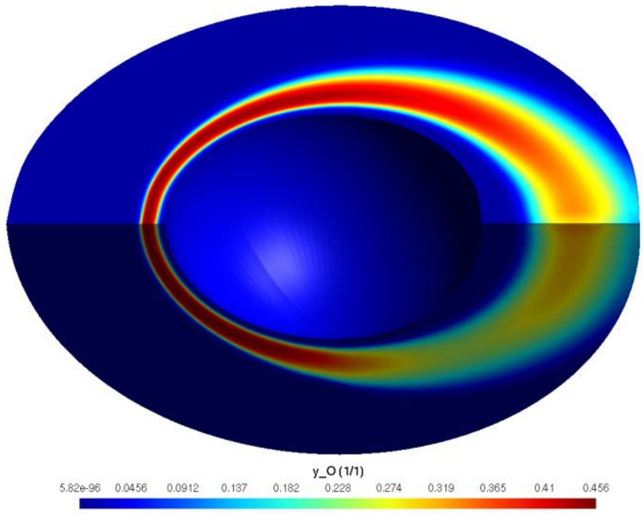


Fig. 4. Atomic oxygen concentration

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