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The implicit fully coupled numerical method for flows in thermochemical nonequilibrium

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The implicit fully coupled numerical method for flows in thermochemical nonequilibrium

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Abstract. A new effective implicit fully coupled numerical method to compute a high-speed flowfield that is in thermochemical nonequilibrium has been developed. Such a flowfield is described by coupled partial differential equations for the conservation of mass, momentum, total energy, vibrational energies, rotational energy, mass conservation for each species, etc. The total number of equations can be very large, which greatly complicates the solution of general finite volume vector equation when using the standard fully implicit approach. The proposed method allows us to reduce operations with block tridiagonal matrices to inversion of 4x4 matrices and trivial matrix multiplication operations. Moreover, the approximation factorization error is minimized. The numerical procedures were applied to solve chemical and thermal nonequilibrium flow past a sphere body at Mach 27 and chemically nonequilibrium heterogeneous flow in the channel of a combined ramjet with a solid fuel gas generator. The results indicate that new method is 4-5 times more efficient than the standard fully implicit method.

1. Introduction

It is known that in chemically and thermally nonequilibrium flows, the characteristic times of the main processes can differ from each other by several orders of magnitude. Therefore, the system of equations is stiff, and its numerical solution requires large computer resources.

Implicit numerical methods are most often used to solve the stiffness problem. The use of these methods leads to the need of multiple inversion of matrices having a dimension corresponding to the number of equations at each time step in each grid node. In the case when the system contains a very large number of equations (tens or even hundreds), the direct use of fully implicit methods may become ineffective.

2. Numerical method

The basic system of equations describing the flow of a chemically and thermally nonequilibrium gas includes the equations of continuity, momentum, total energy, rotational energy, vibrational energies, electron energy, and mass conservation equations for each species. The fully implicit finite-volume representation of this system of equations is as follows [1,2]:

$$\mathbf{A}_{i,j}\delta\mathbf{U}_{i,j}^{n+1}+\mathbf{B}_{i,j}\delta\mathbf{U}_{i,j+1}^{n+1}+\mathbf{C}_{i,j}\delta\mathbf{U}_{i,j-1}^{n+1}+\mathbf{D}_{i,j}\delta\mathbf{U}_{i+1,j}^{n+1}+\mathbf{E}_{i,j}\delta\mathbf{U}_{i-1,j}^{n+1}=\Delta\mathbf{U}_{i,j}^{n+1}+\Delta t\mathbf{H}^{n}, \quad (1)$$

where $\delta\mathbf{U}_{i,j}^{n+1}$ is an implicit solution change of the main vector $\mathbf{U}$ at grid point i,j during the interval from time $n\Delta t$ to time $(n+1)\Delta t$; $\Delta\mathbf{U}_{i,j}^{n+1}$ is an explicit solution change of the main vector $\mathbf{U}$ due to

viscous and inviscid fluxes; **H** is the source vector; $\mathbf{A}_{i,j}, \mathbf{B}_{i,j}, \mathbf{C}_{i,j}, \mathbf{D}_{i,j}, \mathbf{E}_{i,j}$ are block matrix elements whose size coincides with a number of equations in the main system. Here, to reduce the recording volume, a 2D case is presented; extension to a 3D problem does not introduce fundamental differences in the implementation of the method.

To obtain the system (1), Roe method [3] for splitting inviscid fluxes and Tysinger and Caughey approach [4] for implicit viscous fluxes were used.

The matrix $\mathbf{A}_{i,j}$ can be represented as $\mathbf{A}_{i,j} = \mathbf{I} + \alpha\Delta t\, \mathbf{a}_{i,j} - \alpha\Delta t \left(\partial\mathbf{H}/\partial\mathbf{U}\right)_{i,j}^{n}$, where **I** is the identity matrix; $\partial\mathbf{H}/\partial\mathbf{U}$ is the Jacobi matrix; the $\alpha \geq 0.5$ determines the order of accuracy of the time derivative. For $\alpha = 0.5$ the time derivative is centered, Crank-Nicholson like, and second order accurate, otherwise it is of first order. At $\alpha = 1$ the method is fully implicit and for $a > 1$ it is over relaxed, but may have better convergence properties depending on the particular simulation.

The source **H** is associated with transitions between different energy modes, rates of formation of chemical components, etc. The time scales of these processes are very small and can cause the equation set to be extremely stiff. The cost of using fully implicit approach is expensive time steps and complicated coding. For example, if turbulent gas mixture contains 13 species, there are 9 vibrational modes and 1 rotational mode, we have the system of 28 equations: 1 continuity equation, 2 momentum equations, 1 total energy equation, 12 species equations, 9 vibrational energy equation, 1 rotational energy equation and 2 turbulence model equations. For this particular formulation, block tridiagonal solves are required, where each block has dimensions of 28x28. Another cost of the large equation set and fully implicit approach is a high memory requirement.

Therefore, we need to use a more economical approach, not associated with multiple inversions of 28x28 matrices at each grid point.

In [5], a convenient method for numerical implementation was proposed, based on sequential alternation at two half-steps in time of the explicit and implicit representation of viscous/inviscid members of the system and source. It is easy to show that this approach is equivalent to the following factorization of system (1):

$$\left[\mathbf{I} - 0.5\Delta t\left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}}\right)_{i,j}^{n}\right]\left[\left(\mathbf{I} + \alpha\Delta t\, \mathbf{a}_{i,j}\right)\delta\mathbf{U}_{i,j}^{n+1} + \mathbf{B}_{i,j}\delta\mathbf{U}_{i,j+1}^{n+1} + \mathbf{C}_{i,j}\delta\mathbf{U}_{i,j-1}^{n+1} + \mathbf{D}_{i,j}\delta\mathbf{U}_{i+1,j}^{n+1} + \mathbf{E}_{i,j}\delta\mathbf{U}_{i-1,j}^{n+1}\right] \quad (2)$$
$$= \Delta\mathbf{U}_{j}^{n+1} + \Delta t\mathbf{H}^{n}$$

The main advantage of this approach is that all the matrices that appear in the right bracket of the left side of equation (2), $\mathbf{a}_{i,j}, \mathbf{B}_{i,j}, \mathbf{C}_{i,j}, \mathbf{D}_{i,j}, \mathbf{E}_{i,j}$ and most importantly the matrices that appear in intermediate calculations, have a common block form:

$$\mathbf{\Phi} = \begin{pmatrix} \mathbf{\Phi}_{11} & \mathbf{\Phi}_{12} \\ \mathbf{\Phi}_{21} & \mathbf{\Phi}_{22} \end{pmatrix} = \begin{pmatrix} \mathbf{\Phi}_{11} & \mathbf{0} \\ \mathbf{\Phi}_{21} & \mathbf{D} \end{pmatrix}, \quad (3)$$

where the matrix blocks have the following dimensions: $\mathbf{\Phi}_{11}$ - 4x4; $\mathbf{\Phi}_{21}$ - N_ax4; **D** - diagonal matrix of size N_a. Here N_a is the number of additional equations, not including 4 basic equations (continuity, 2 momentum and total energy).

The main advantages of a matrix of the form (3) are as follows:

1) its inversion is reduced to a single inversion of the matrix $\mathbf{A}_{11}$ and trivial operations of matrix multiplication (Frobenius formula):

$$\mathbf{\Phi}^{-1} = \begin{pmatrix} \mathbf{\Phi}_{11}^{-1} & \mathbf{0} \\ -\mathbf{D}^{-1}\mathbf{\Phi}_{21}\mathbf{\Phi}_{11}^{-1} & \mathbf{D}^{-1} \end{pmatrix} \quad (4)$$

2) any necessary operations with such a matrix (inversion, multiplication) do not change its shape, i.e. the block $\mathbf{\Phi}_{12}$ remains zero, and the block $\mathbf{\Phi}_{22}$ remains a diagonal matrix.

Thus, even a significant increase in the number of additional equations (i.e., the number of chemical components) does not necessitate the use of large computer resources.

After multiplying the matrices, we obtain on the left-hand side of (2)

$$\left[\mathbf{I}+\alpha\Delta t\,\mathbf{a}_{i,j}-0.5\Delta t\left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}}\right)^{n}_{i,j}-0.5\alpha\left(\Delta t\right)^{2}\left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}}\right)^{n}_{i,j}\mathbf{a}_{i,j}\right]\delta\mathbf{U}^{n+1}_{i,j}+\left[\mathbf{I}-0.5\Delta t\left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}}\right)^{n}_{i,j}\right]\mathbf{B}_{i,j}\delta\mathbf{U}^{n+1}_{i,j+1}$$
$$+\left[\mathbf{I}-0.5\Delta t\left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}}\right)^{n}_{i,j}\right]\mathbf{C}_{i,j}\delta\mathbf{U}^{n+1}_{i,j-1}+\left[\mathbf{I}-0.5\Delta t\left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}}\right)^{n}_{i,j}\right]\mathbf{D}_{i,j}\delta\mathbf{U}^{n+1}_{i+1,j}+\left[\mathbf{I}-0.5\Delta t\left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}}\right)^{n}_{i,j}\right]\mathbf{E}_{i,j}\delta\mathbf{U}^{n+1}_{i-1,j} \tag{5}$$
$$=\Delta\mathbf{U}^{n+1}_{i,j}+\Delta t\mathbf{H}\left(\mathbf{U}^{n}_{i,j}\right)$$

A comparison of expressions (5) and (1) shows that the scheme (2) is a rather rough factorization of a fully implicit scheme (1): none of the original matrix elements are returned exactly. The coefficient at $\delta\mathbf{U}^{n+1}_{i,j}$ in (5) differs from the corresponding coefficient in (1) by a value of the second order of smallness. But the remaining members are now dependent on $\left[\mathbf{I}-0.5\Delta t\left(\partial\mathbf{H}/\partial\mathbf{U}\right)^{n}_{i,j}\right]$. This factorization error reduces accuracy and slows algorithm convergence.

The approximation factorization procedure can be significantly improved by reducing the decomposition error.

We can represent the matrix A $\partial\mathbf{H}/\partial\mathbf{U}$ as the sum of diagonal and off-diagonal components:

$$\frac{\partial\mathbf{H}}{\partial\mathbf{U}}=\mathbf{d}+\mathbf{T} \tag{6}$$

and consider the following scheme:

$$\left[\mathbf{I}-\alpha\Delta t\left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}}\right)^{n}_{i,j}\right]\left(\mathbf{I}-\alpha\Delta t\mathbf{d}^{n}_{i,j}\right)^{-1}\times$$
$$\times\left[\left(\mathbf{I}+\alpha\Delta t\,\mathbf{a}_{i,j}-\alpha\Delta t\mathbf{d}^{n}_{i,j}\right)\delta\mathbf{U}^{n+1}_{i,j}+\mathbf{B}_{i,j}\delta\mathbf{U}^{n+1}_{i,j+1}+\mathbf{C}_{i,j}\delta\mathbf{U}^{n+1}_{i,j-1}+\mathbf{D}_{i,j}\delta\mathbf{U}^{n+1}_{i+1,j}+\mathbf{E}_{i,j}\delta\mathbf{U}^{n+1}_{i-1,j}\right]=\Delta\mathbf{U}^{n+1}_{i,j}+\Delta t\mathbf{H}^{n} \tag{7}$$

Here **d** is the diagonal part of the matrix $\partial\mathbf{H}/\partial\mathbf{U}$. In this case, the solution of system (7) is reduced to a single inversion of the matrix associated with the source and to the solution of the system in which all matrices have the form (3). In addition, the matrix $\partial\mathbf{H}/\partial\mathbf{U}$ is easily partitioned into blocks according to physical processes.

Let us analyze this scheme. After multiplying the matrices we get:

$$\left\{\mathbf{I}-\alpha\Delta t\left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}}\right)^{n}_{i,j}+\alpha\Delta t\mathbf{a}_{i,j}-\left(\alpha\Delta t\right)^{2}\mathbf{T}^{n}_{i,j}\left(\mathbf{I}-\alpha\Delta t\,\mathbf{d}^{n}_{i,j}\right)^{-1}\mathbf{a}_{i,j}\right\}\delta\mathbf{U}^{n+1}_{i,j}+\left[\mathbf{I}-\alpha\Delta t\,\mathbf{T}^{n}_{i,j}\left(\mathbf{I}-\alpha\Delta t\,\mathbf{d}^{n}_{i,j}\right)^{-1}\right]\mathbf{B}_{i,j}\delta\mathbf{U}^{n+1}_{i,j+1}$$
$$+\left[\mathbf{I}-\alpha\Delta t\,\mathbf{T}^{n}_{i,j}\left(\mathbf{I}-\alpha\Delta t\,\mathbf{d}^{n}_{i,j}\right)^{-1}\right]\mathbf{C}_{i,j}\delta\mathbf{U}^{n+1}_{i,j-1}+\left[\mathbf{I}-\alpha\Delta t\,\mathbf{T}^{n}_{i,j}\left(\mathbf{I}-\alpha\Delta t\,\mathbf{d}^{n}_{i,j}\right)^{-1}\right]\mathbf{D}_{i,j}\delta\mathbf{U}^{n+1}_{i+1,j} \tag{8}$$
$$+\left[\mathbf{I}-\alpha\Delta t\,\mathbf{T}^{n}_{i,j}\left(\mathbf{I}-\alpha\Delta t\,\mathbf{d}^{n}_{i,j}\right)^{-1}\right]\mathbf{E}_{i,j}\delta\mathbf{U}^{n+1}_{i-1,j}=\Delta\mathbf{U}^{n+1}_{i,j}+\Delta t\mathbf{H}^{n}$$

And again, the coefficient at $\delta\mathbf{U}^{n+1}_{i,j}$ differs from the corresponding coefficient in (1) by a second order value relative to Δt. In addition, if diagonal elements play a decisive role in the matrix $\partial\mathbf{H}/\partial\mathbf{U}$, then

$$\left\|\alpha\Delta t\mathbf{T}^{n}_{i,j}\left(\mathbf{I}-\alpha\Delta t\mathbf{D}^{n}_{i,j}\right)^{-1}\right\|=\left\|\mathbf{T}^{n}_{i,j}\left(\mathbf{I}/\left(\alpha\Delta t\right)-\mathbf{D}^{n}_{i,j}\right)^{-1}\right\|=\left\|\mathbf{T}^{n}_{i,j}\left(\mathbf{I}/\left(\alpha\Delta t\right)-\mathbf{D}^{n}_{i,j}\right)^{-1}\right\|=\frac{\left\|\mathbf{T}^{n}_{i,j}\right\|}{\left\|\mathbf{I}/\left(\alpha\Delta t\right)-\mathbf{D}^{n}_{i,j}\right\|}\ll 1 \tag{9}$$

Thus, with sufficient accuracy, equation (8) is transformed into

$$\left\{\mathbf{I}-\alpha\Delta t\left(\frac{\partial\mathbf{H}}{\partial\mathbf{U}}\right)^{n}_{i,j}+\alpha\Delta t\mathbf{a}_{i,j}\right\}\delta\mathbf{U}^{n+1}_{i,j}+\mathbf{B}_{i,j}\delta\mathbf{U}^{n+1}_{i,j+1}+\mathbf{C}_{i,j}\delta\mathbf{U}^{n+1}_{i,j-1}+\mathbf{D}_{i,j}\delta\mathbf{U}^{n+1}_{i+1,j}+\mathbf{E}_{i,j}\delta\mathbf{U}^{n+1}_{i-1,j}=\Delta\mathbf{U}^{n+1}_{i,j}+\Delta t\mathbf{H}^{n} \tag{10}$$

This expression exactly matches the fully implicit scheme (1).

Thus, we obtain an implicit numerical scheme, in which, on the one hand, the problem of stiffness is completely solved (the scheme is unconditionally stable and fully coupled); on the other hand, the number of matrix inverses is reduced, and the matrices themselves are factorized into smaller ones, and their inversion requires significantly less computer resources than in a fully implicit scheme.

3. Numerical results

To test the numerical method just presented, we calculated a series of problems.

3.1. Test 1

Simulation of a nonequilibrium flow past the sphere head of a hypersonic aircraft was the first test case. Mach number M = 27, flight altitude = 75 km; 11 chemical components, 3 vibrational energy modes, 1 general rotational energy mode, zero catalytic activity.

The following boundary conditions were used: the radius of the spherical part R = 0.05m; freestream speed u_e = 7800 m/s; temperature and pressure in the surrounding space T_e = 208.4K, p_e = 2.388Pa; the standard atmospheric composition for a given altitude. Wall temperature T_w = 700K.

Figure 1 shows the heat flux density distribution on the surface of the head. Curve 1 - the calculation using a fully implicit scheme (equation (1)); curve 2 - the calculation using an implicit scheme with factorization (7).

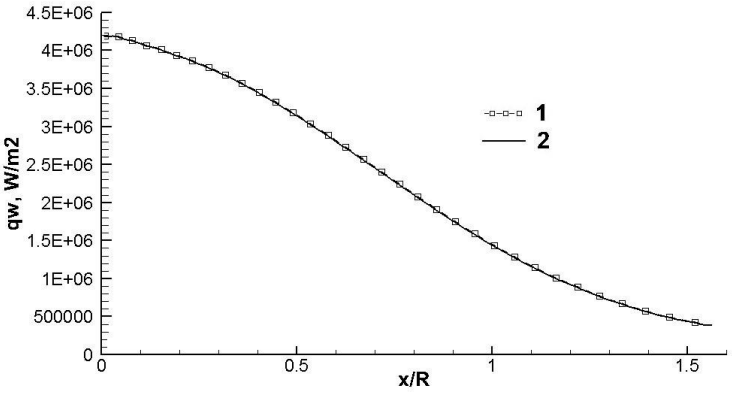

Figure 1. Heat flux density distribution on the surface of the head

Obviously, the results of both calculations completely coincide.

3.2. Test 2.

Chemically nonequilibrium heterogeneous flow in the channel of a combined ramjet with a solid fuel gas generator (Figure 1). Flight speed M = 7, altitude = 40 km; 14 species taken into account.

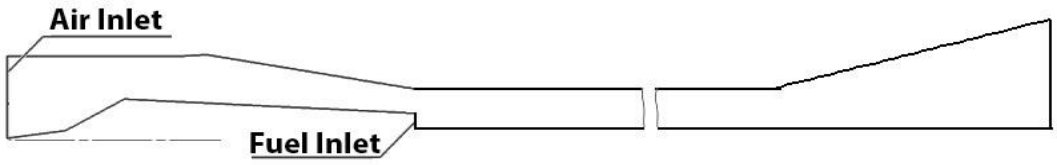

Figure 2. Schematic drawing of the combined ramjet

The following boundary conditions at the air inlet were used: flight speed u_e = 2222 m/s; ambient temperature and pressure T_e = 250.4K, p_e = 287.143Pa; the standard atmospheric composition for a given altitude. The parameters at the outlet of the gas generator (Fuel Inlet) are presented in table 1.

Table 1. Fuel Inlet parameters

Velocity, m/s	Temperature, K	Pressure, Pa	H	H2	H2O	CO	CO2	HCl	N2
1582	2026	8.E4	0.3438E-3	0.3775	0.1232E-4	0.3635	0.3157E-5	0.57227E-2	0.24203

The composition is set in mole fractions. The length of the combustion chamber = 21.5 m.
Figires 3,4 show the pressure distribution on the wall of the combustion chamber (Figure 3 – the calculation with considering the chemical reactions, Figure 4 - calculation without considering the chemical reactions)

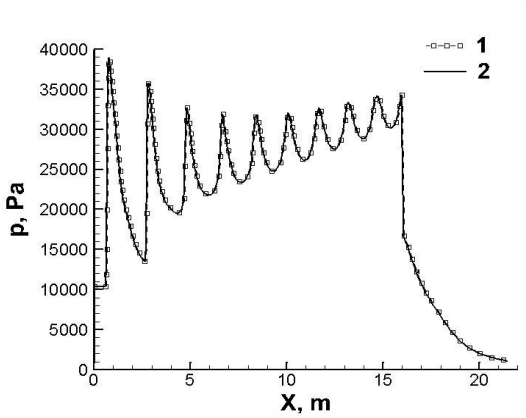

Figure 3. Pressure distribution on the wall of the combustion chamber (chemically reacting case)

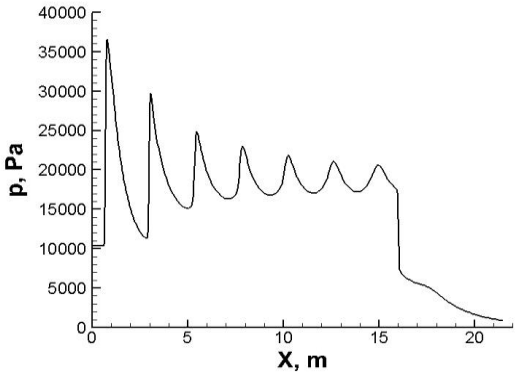

Figure 4. Pressure distribution on the wall of the combustion chamber (chemical reactions are not taken into account)

In Figure 3: curve 1 — the calculation using a implicit scheme Eq.(1); curve 2 - calculation using an implicit scheme with factorization (7). Both calculations are in good agreement.

Comparison of the effectiveness of various numerical schemes is presented in table 2:

Table 2. Comparison of the effectiveness of various numerical schemes

Scheme	Number of iterations	Computer time spent on one iteration, in relation to a standard fully implicit scheme
Fully implicit scheme (1)	600-800	1
Half-step alternating scheme (2)	1000-1500	0.2 - 0.25
Modified scheme (7)	650-900	0.2 - 0.25

Thus, the proposed scheme allows us to reduce the calculation time by 4-5 times in comparison with a fully implicit scheme. With a larger number of components and energy modes, this difference will be even more significant.

4. Conclusions

An implicit fully coupled numerical scheme has been developed for solving equations describing the flow of a thermochemically nonequilibrium gas. Using this numerical method, on the one hand, helped

to completely solve the stiffness problem (the scheme is unconditionally stable and fully coupled), and on the other hand, to reduce the number of matrix inversion. The matrices themselves are factorized into smaller ones, and their inversion requires significantly less computer resources than using a purely implicit scheme. The performed test calculations showed that the proposed numerical scheme is highly efficient.

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