The Application of Krylov Implicit Integration Factor Method in Numerical Simulation of Deflagration to Detonation

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1 Introduction

The mechanism of deflagration-to-detonation transition (DDT) for combustible gas is very intricate, which complicates direct numerical simulation. The stiff reactive terms comprising in the reactive Navier-Stokes equations require very small time step size so as to ensure the stability of explicit scheme. Although implicit scheme can be employed to overcome such limitation, solving large non-linear equations increases the computational cost dramatically. Implicit integration factor (IIF) methods, performing the time evolution via evaluation of an exponential function of the corresponding matrix, are classical and efficient time discretization approaches for solving time-dependent partial differential equations (PDEs). The IIF methods not only eliminate the stability constrain, but also substantially reduce time direction numerical errors from the high order derivatives[1-4]. Zhang et al. [5] developed a class of efficient implicit integration factor (IIF) methods for solving systems with stiff terms. The size of the nonlinear system arising from the implicit treatment is merely dependent on the number of the original PDEs. In theory, the improved methods can achieve arbitrary order accuracy and large stability region thanks to the implicit nature of the schemes. For multi-dimensional problems, compact implicit integration factor (cIIF) based on rectangular mesh[6] and Krylov implicit integration factor (KIIF) based on unstructured mesh[7] was presented. Liu[8] proposed a generalized cIIF method with adaptive mesh refinement (AMR) satisfying the excellent stability condition for curvilinear coordinates such as polar and spherical coordinates, which has similar computational efficiency and stability properties to the cIIF in Cartesian coordinate. Zhang[9] further analyzed the numerical stability and truncation errors of the KIIF method to validate and demonstrate the broad prospect for solving nonlinear PDEs.

In the paper, the KIIF method is extended to investigate the DDT mechanism using the reactive Navier-Stokes equations with source terms. Time discretization is performed by the KIIF method. The stiff reactive terms utilize implicit scheme, and the non-stiff advection-diffusion terms use explicit scheme. Large time-step size is needed, which drastically reduces the number of computational steps required in the simulation. On the other hand, mapping the large sparse matrix to the Krylov subspace greatly decreases the dimensions of equations and thus saves the computational cost.

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2 Governing equations

The governing equations used for investigating DDT are the two-dimensional Navier-Stokes equations with source terms as follows

$$\frac{\partial U}{\partial t}+\frac{\partial F(U)}{\partial x}+\frac{\partial G(U)}{\partial y}=\mathbf{Dif}+S \tag{1}$$

$$U=\left(\rho,\rho u,\rho v,\rho e,\rho Y\right)^T$$

$$F(U)=\left(\rho u,\rho u^2+p,\rho uv,\rho u(e+p/\rho),\rho uY\right)^T$$

$$G(U)=\left(\rho v,\rho vu,\rho v^2+p,\rho v(e+p/\rho),\rho vY\right)^T$$

$$S(U)=\left(0,0,0,0,-\dot{\omega}_F\right)^T$$

$$\mathbf{Dif}=[\mathrm{dif}_1,\mathrm{dif}_2,\mathrm{dif}_3,\mathrm{dif}_4,\mathrm{dif}_5]^T$$

$$e=\frac{R_pT}{(\gamma-1)m}+YQ+\frac{1}{2}(u^2+v^2)$$

$$\mathrm{Dif}_1=0$$

$$\mathrm{Dif}_2=\frac{\partial}{\partial x}(\mu(\frac{4}{3}\frac{\partial u}{\partial x}-\frac{2}{3}\frac{\partial v}{\partial y}))+\frac{\partial}{\partial y}(\mu(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}))$$

$$\mathrm{Dif}_3=\frac{\partial}{\partial x}(\mu(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}))+\frac{\partial}{\partial y}(\mu(\frac{4}{3}\frac{\partial v}{\partial y}-\frac{2}{3}\frac{\partial u}{\partial x}))$$

$$\mathrm{Dif}_4=\frac{\partial}{\partial x}(\frac{\mu C_p}{\mathrm{Pr}}\frac{\partial T}{\partial x}+\frac{\mu Q}{\mathrm{Sc}}\frac{\partial Y}{\partial x}+u\mu(\frac{4}{3}\frac{\partial u}{\partial x}-\frac{2}{3}\frac{\partial v}{\partial y})+v\mu(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}))$$
$$+\frac{\partial}{\partial y}(\frac{\mu C_p}{\mathrm{Pr}}\frac{\partial T}{\partial y}+\frac{\mu Q}{\mathrm{Sc}}\frac{\partial Y}{\partial y}+u\mu(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y})+v\mu(\frac{4}{3}\frac{\partial v}{\partial y}-\frac{2}{3}\frac{\partial u}{\partial x}))$$

$$\mathrm{Dif}_5=\frac{\partial}{\partial x}(\frac{\mu}{\mathrm{Sc}}\frac{\partial Y}{\partial x})+\frac{\partial}{\partial y}(\frac{\mu}{\mathrm{Sc}}\frac{\partial Y}{\partial y})$$

$$\dot{\omega}_F=A\rho(1-Y)\mathrm{e}^{-\frac{Ea}{R_pT}}$$

where, ρ , T , p , e , Q , Y , u and v are density, temperature, pressure, internal energy, the heat of reaction, the reactant mass fraction, and two Cartesian components of the velocity vector, respectively.

3 Numerical method

An explicit-implicit scheme is presented to solve stiff problems, and the strategy mapping the large sparse matrix to the Krylov subspace is used to solve large equations. In spatial discretization, the weighted essentially non-oscillatory scheme is needed to discretize the advection terms. The second or fourth order central finite difference scheme is used to discretize the diffusion terms. Krylov implicit integration factor method is used for time discretization.

3.1 Spatial discretization

1. In this section, we use the third order finite difference WENO scheme to discretize the nonlinear advection terms. We at first perform Lax-Friedrichs flux splitting

$$f^{\pm}(U)=\frac{1}{2}\left(f(U)\pm\alpha U\right)$$

Where $\alpha=\max\left|f'(U)\right|$

$$\left(\frac{\partial f(U)}{\partial x}\right)_{ij}=\frac{1}{\Delta x}\left(\hat{f}^{+}_{i+1/2,j}-\hat{f}^{+}_{i-1/2,j}\right)+\frac{1}{\Delta x}\left(\hat{f}^{-}_{i+1/2,j}-\hat{f}^{-}_{i-1/2,j}\right)$$

Where $\hat{f}^{+}_{i+1/2} = \omega_0\left[\frac{1}{2}f^{+}(U_i)+\frac{1}{2}f^{+}(U_{i+1})\right]+\omega_1\left[-\frac{1}{2}f^{+}(U_{i-1})+\frac{3}{2}f^{+}(U_i)\right]$

$\omega_r = \frac{a_r}{a_0+a_1}$, $a_r = \frac{d_r}{(\varepsilon+\beta_r)^2}$, $r = 0,1$

$d_0 = \frac{2}{3}$, $d_1 = \frac{1}{3}$, $\beta_0 = (f(U_{i+1})-f(U_i))^2$, $\beta_1 = (f(U_i)-f(U_{i-1}))^2$

Similar procedures are applied to the other directions for $\frac{\partial g(U)}{\partial y}$.

2. The diffusion terms are discretized by central finite difference scheme. For example, a second order approximation to a nonlinear diffusion term Dif_2 has the form

$$\mathrm{Dif}_2 = \frac{\partial}{\partial x}\left(\mu\left(\frac{4}{3}\frac{\partial u}{\partial x}-\frac{2}{3}\frac{\partial v}{\partial y}\right)\right)+\frac{\partial}{\partial y}\left(\mu\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)\right)$$

$$\mu\frac{\left(\frac{4}{3}\frac{\partial u}{\partial x}-\frac{2}{3}\frac{\partial v}{\partial y}\right)_{i+\frac{1}{2},j}-\left(\frac{4}{3}\frac{\partial u}{\partial x}-\frac{2}{3}\frac{\partial v}{\partial y}\right)_{i-\frac{1}{2},j}}{\Delta x}+\mu\frac{\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)_{i,j+\frac{1}{2}}-\left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)_{i,j-\frac{1}{2}}}{\Delta y}$$

$$=\mu\frac{\left(\frac{4}{3}\frac{u_{i+1,j}-u_{i,j}}{\Delta x}-\frac{2}{3}\frac{v_{i+\frac{1}{2},j+\frac{1}{2}}-v_{i+\frac{1}{2},j-\frac{1}{2}}}{\Delta y}\right)-\left(\frac{4}{3}\frac{u_{i,j}-u_{i-1,j}}{\Delta x}-\frac{2}{3}\frac{v_{i-\frac{1}{2},j+\frac{1}{2}}-v_{i-\frac{1}{2},j-\frac{1}{2}}}{\Delta y}\right)}{\Delta x}$$

$$+\mu\frac{\left(\frac{v_{i+\frac{1}{2},j+\frac{1}{2}}-v_{i-\frac{1}{2},j+\frac{1}{2}}}{\Delta x}+\frac{u_{i,j+1}-u_{i,j}}{\Delta y}\right)-\left(\frac{v_{i+\frac{1}{2},j-\frac{1}{2}}-v_{i-\frac{1}{2},j-\frac{1}{2}}}{\Delta x}+\frac{u_{i,j}-u_{i,j-1}}{\Delta y}\right)}{\Delta y}$$

Similar procedures are applied to other terms.

Thus we obtain the semi-discretized ODE system from (1)

$$\frac{\mathrm{d}\vec{U}}{\mathrm{d}t} = F_d(\vec{U})+F_a(\vec{U})+R(\vec{U}) \tag{2}$$

Where $\vec{U} = (U_{ij})_{1\le i\le N_1,1\le j\le N_2}$, $F_d(\vec{U})$ is the approximation for the diffusion terms by the finite difference schemes, $F_a(\vec{U})$ is the approximation for the diffusion terms by the finite difference schemes, ， $R(\vec{U})$ is the nonlinear reaction term, N_1 and , N_2 are the total number of grid points in direction x and y, respectively.

3.2 Time discretization

We construct Krylov IIF method for (2). Multiply the equation (2) by the integration factor e^{-Ct}, where C is the Jacobian matrix of $\frac{\partial F_d(\vec{U})}{\partial\vec{U}}$. Then integrate over one time step from t_n to $t_{n+1} = t_n+\Delta t_n$.

$$\int_{t_n}^{t_{n+1}} e^{-Ct}\frac{\mathrm{d}\vec{U}}{\mathrm{d}t}\mathrm{d}t = \int_{t_n}^{t_{n+1}} e^{-Ct}\left[F_d(\vec{U})+F_a(\vec{U})+R(\vec{U})\right]\mathrm{d}t\,.$$

Integrating by parts and change of variable, we obtain

$$\vec{U}_{n+1} = e^{C_n\Delta t_n}\vec{U}_n+e^{C_n\Delta t_n}\int_0^{\Delta t_n} e^{-C_n\tau}\left[F(\vec{U}(t_n+\tau))+R(\vec{U}(t_n+\tau))\right]\mathrm{d}\tau$$

where $F(\vec{U}(t_n+\tau)) = F_d(\vec{U}(t_n+\tau))-C\vec{U}(t_n+\tau)+F_a(\vec{U}(t_n+\tau))$.

Denote $\tau_1 = \Delta t$, $\tau_0 = 0$, $\tau_i = -\sum_{k=i}^{-1}\Delta t_{n+k}$ $(i = -1,-2,\cdots,1-r)$,

The interpolation points are represented by $t_{n+i} = t_n + \tau_i$, $i = 1, 0, -1, \cdots, 1-r$. The first r points $\{t_{n+i} : i = 1, 0, -1, -2, \cdots, 2-r\}$ are used for an implicit approximation of the nonlinear reaction term:

$$e^{C_n \Delta t_n} \int_0^{\Delta t_n} e^{-C_n \tau} R(\vec{U}(t_n + \tau))\, \mathrm{d}\tau \approx \sum_{i=2-r}^{1} e^{C_n(\Delta t_n - \tau_i)} R(\vec{U}_{n+i}) \int_0^{\Delta t_n} \prod_{\substack{j=2-r \\ j \neq i}}^{1} \frac{\tau - \tau_j}{\tau_i - \tau_j} \mathrm{d}\tau .$$

And other terms are approximated explicitly:

$$e^{C_n \Delta t_n} \int_0^{\Delta t_n} e^{-C_n \tau} F(\vec{U}(t_n + \tau))\, \mathrm{d}\tau \approx \sum_{i=1-r}^{0} e^{C_n(\Delta t_n - \tau_i)} F(\vec{U}_{n+i}) \int_0^{\Delta t_n} \prod_{\substack{j=1-r \\ j \neq i}}^{0} \frac{\tau - \tau_j}{\tau_i - \tau_j} \mathrm{d}\tau .$$

Then we attain the *r*-th order IIF scheme

$$\vec{U}_{n+1} = e^{C_n \Delta t_n} \vec{U}_n + \sum_{i=2-r}^{1} e^{C_n(\Delta t_n - \tau_i)} R(\vec{U}_{n+i}) \int_0^{\Delta t_n} \prod_{\substack{j=2-r \\ j \neq i}}^{1} \frac{\tau - \tau_j}{\tau_i - \tau_j} \mathrm{d}\tau + \sum_{i=1-r}^{0} e^{C_n(\Delta t_n - \tau_i)} F(\vec{U}_{n+i}) \int_0^{\Delta t_n} \prod_{\substack{j=1-r \\ j \neq i}}^{0} \frac{\tau - \tau_j}{\tau_i - \tau_j} \mathrm{d}\tau$$

that is

$$\vec{U}_{n+1} = e^{C_n \Delta t_n} \vec{U}_n + \Delta t_n \left[\alpha_{n+1} R(\vec{U}_{n+1}) + \sum_{i=2-r}^{0} \alpha_{n+i} e^{C_n(\Delta t_n - \tau_i)} R(\vec{U}_{n+i}) + \sum_{i=1-r}^{0} \beta_{n+i} e^{C_n(\Delta t_n - \tau_i)} F(\vec{U}_{n+i}) \right]$$

where $\alpha_{n+i} = \dfrac{1}{\Delta t_n} \int_0^{\Delta t_n} \prod_{\substack{j=2-r \\ j \neq i}}^{1} \dfrac{\tau - \tau_j}{\tau_i - \tau_j} \mathrm{d}\tau$, $i = 1, 0, -1, -2, \cdots, 2-r$

$$\beta_{n+i} = \frac{1}{\Delta t_n} \int_0^{\Delta t_n} \prod_{\substack{j=1-r \\ j \neq i}}^{0} \frac{\tau - \tau_j}{\tau_i - \tau_j} \mathrm{d}\tau , \quad i = 0, -1, -2, \cdots, 1-r$$

For example, the second order scheme (IIF2) is

$$\vec{U}_{n+1} = e^{C_n \Delta t_n} \vec{U}_n + \Delta t_n \left[\alpha_{n+1} R(\vec{U}_{n+1}) + \alpha_n e^{C_n \Delta t_n} R(\vec{U}_n) + \beta_n e^{C_n \Delta t_n} F(\vec{U}_n) + \beta_{n-1} e^{C_n(\Delta t_n + \Delta t_{n-1})} F(\vec{U}_{n-1}) \right],$$

where $\alpha_n = \dfrac{1}{2}$, $\alpha_{n+1} = \dfrac{1}{2}$, $\beta_{n-1} = \dfrac{-\Delta t_n}{2\Delta t_{n-1}}$, $\beta_n = \dfrac{1}{\Delta t_{n-1}} \left(\dfrac{\Delta t_n}{2} + \Delta t_{n-1} \right)$.

3.3 Krylov IIF schemes

It is difficult to calculate $e^{C_n \Delta t_n}$ because of the large sparse matrix *C*. We project it to the Krylov subspace

$$K_M = \mathrm{span}\left\{ \vec{v}, C\vec{v}, C^2\vec{v}, \cdots, C^{M-1}\vec{v} \right\}.$$

The dimension *M* of the Krylov subspace is much smaller than the dimension *N* of the large sparse matrix *C*. So we take *M* =25 for different *N*, and the accuracy is satisfied in our simulation[9]. First, we generate the Krylov subspace by the Arnoldi algorithm as follows.

1. Compute the initial unite vector: $v_1 = \dfrac{v}{\|v\|_2}$

2. Perform iterations: *j* =1,2, ..., *M*, compute the vector $w = Cv_j$

   Do i=1,2,..., j

   (1) Compute the inner product $h_{ij} = (w, v_i)$.

   (2) Compute the vector $w = w - h_{ij} v_i$

   (3) Compute $h_{j+1,j} = \|w\|_2$

   (4) If $h_{j+1,j} = 0$, then

   stop the iteration.

   else

   compute the next basis vector $v_{j+1} = w / h_{j+1,j}$.

Then we obtain an upper Hessenberg matrix $H_M = \begin{pmatrix} h_{11} & h_{12} & h_{13} & \cdots & h_{1,m-1} & h_{1m} \\ h_{21} & h_{22} & h_{23} & \cdots & h_{2,m-1} & h_{2m} \\ 0 & h_{32} & h_{33} & \cdots & h_{3,m-1} & h_{3m} \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ddots & h_{m-1,m-1} & h_{m-1,m} \\ 0 & 0 & 0 & \cdots & h_{m,m-1} & h_{mm} \end{pmatrix}$ satisfying

$$h_{i+1,i}v_{i+1} = Cv_i - h_{i1}v_1 - h_{i2}v_2 - \cdots - h_{ii}v_i .$$

That is

$$Cv_i = h_{i1}v_1 + h_{i2}v_2 + \cdots + h_{ii}v_i + h_{i+1,i}v_{i+1} = (v_1, v_2, \cdots, v_{i+1}) \begin{pmatrix} h_{i1} \\ h_{i2} \\ \vdots \\ h_{i+1,i} \end{pmatrix}$$

then, $C(v_1, v_2, \cdots, v_m) = (v_1, v_2, \cdots, v_{i+1})H_M$.

Denote $V_M = (v_1, v_2, \cdots, v_m)$, we have $CV_M = V_M H_M$,

$$H_M = \begin{pmatrix} h_{11} & h_{12} & h_{13} & \cdots & h_{1,m-1} & h_{1m} \\ h_{21} & h_{22} & h_{23} & \cdots & h_{2,m-1} & h_{2m} \\ 0 & h_{32} & h_{33} & \cdots & h_{3,m-1} & h_{3m} \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ddots & h_{m-1,m-1} & h_{m-1,m} \\ 0 & 0 & 0 & \cdots & h_{m,m-1} & h_{mm} \end{pmatrix} = V_M^T C V_M$$

Since V_M is orthonormal, the vector $V_M V_M^T e^{C\Delta t}v$ is the orthogonal projection of $e^{C\Delta t}v$ on K_M , that is to say, it is the closest approximation to $e^{C\Delta t}v$ from K_M . Therefore,

$$e^{C\Delta t}v \approx V_M V_M^T e^{C\Delta t}v = \beta V_M V_M^T e^{C\Delta t}v_1 = \beta V_M V_M^T e^{C\Delta t}V_M e_1 = \beta V_M e^{H_M \Delta t}e_1$$

where $\beta = \|v\|_2$, e_1 denotes the first column of M . Thus the large $e^{C\Delta t}v$ matrix exponential problem is replaced by a much smaller $e^{H_M \Delta t}$ problem. The smaller matrix exponential $e^{H_M \Delta t}$ is computed using a scaling and squaring algorithm[10], involving less computational cost $O(M^2)$.

4 Numerical simulation

The width of the tube full of premixed mixture is $20L_f$. The left side is closed and the other side open. Both the upper and bottom walls are non-slip. A planar flame resulting from a weak ignition is located on the left. In the unreacted mixture, initial velocity, temperature and pressure are 0.0m/s, 300K and 1atm, respectively. Figure 1 shows the temperature evolutions in the reactive process. It illustrates that flame initially accelerates due to the expansion of hot products. The flow velocity constantly changes along the transverse direction, and increases gradually from the wall to the center. The perturbations behind the flame front propagate into upstream, thus change the initial value in unreacted mixture. Flame stretch expands the flame surface, hence more chemical energy is released. As flame propagates, the gas flow ahead of the flame front accelerates constantly.

5 Conclusion

In the paper, Krylov implicit integration factor is used in the numerical simulation of flame acceleration and deflagration to detonation transition. The numerical results further demonstrate and validate the correction and effectiveness of the novel theoretical analysis used in the reactive Navier-Stokes equations. Because the stiff reactive terms are discretized by implicit scheme, large time step can be utilized to dramatically save computational cost. The method presented in the paper is designed

to offer a novel strategy to numerically investigate the intrinsic mechanism of flame acceleration and deflagration to detonation transition using direct numerical simulation with low computation cost. One can directly extend the method to the three-dimensional reactive Navier-Stokes equations with detailed chemical reaction model, which certainly make the advantage of the method more obvious.

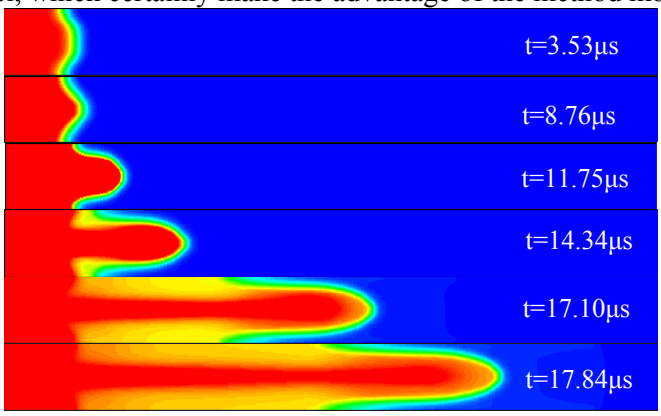

Figure 1 Numerical simulation of flame acceleration

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