

# Applications of Dual Time Stepping to Fully Implicit Runge-Kutta Schemes for Unsteady Flow Calculations

Antony Jameson

Aerospace Computing Laboratory  
Department of Aeronautics and Astronautics  
Stanford University

University of Texas, Austin,  
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# Introduction

## Integral Conservation Law

Consider the Euler equations for gas dynamics can be expressed in conservation law form

$$\mathbf{w} = \begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ \rho E \end{bmatrix},$$

where  $\rho$  is the density,  $u_i$  are the velocity components and  $E$  is the total energy. The flux vectors are

$$\mathbf{f}_i = u_i \mathbf{w} + p \begin{bmatrix} 0 \\ \delta_{i1} \\ \delta_{i2} \\ \delta_{i3} \\ u_i \end{bmatrix}$$

where the pressure is

$$p = (\gamma - 1)\rho(E - u_i u_i).$$

## Integral Conservation Law

A semi-discrete finite volume scheme is obtained directly approximating the integral form on each computational cell

$$\frac{d}{dt} \int_{\text{cell}} \mathbf{w} dV + \int_{\text{cell boundary}} \mathbf{n}_i \mathbf{f}_i dS = 0,$$

where  $\mathbf{n}_i$  are the components of the unit normal to the cell boundary. This leads to a semi-discrete equation with the general form

$$V \frac{d\mathbf{w}}{dt} + R(\mathbf{w}) = 0 \quad (1)$$

where  $\mathbf{w}$  now denotes the average value of the state in the cell.  $V$  is the cell volume, or in the two dimensional case, the cell area.  $R(\mathbf{w})$  is the residual resulting from the space discretization.

# Paradox of Fast Steady State Solver



Figure 1: Paradox of fast steady state solver.

## Paradox of Fast Steady State Solver

In the early days of CFD, it was commonly assumed that in order to obtain fast convergence to a steady state, it would be necessary to use an implicit scheme which allowed large time steps. Any implicit scheme, however, such as the backward Euler scheme

$$w^{n+1} = w^n - \Delta t R(w^{n+1})$$

with the superscript  $n$  denoting the time level, requires the solution of a large number of coupled nonlinear equations which have the same complexity as the steady state problem,

$$R(w) = 0.$$

Accordingly, a fast steady state solver is an essential building block for an implicit scheme. This leads to a circular situation. We need an implicit scheme for fast convergence to a steady state, but we need a fast steady state solver to build an implicit scheme. This situation is reminiscent of the scene shown in figure 1 of two dragons, each consuming the other's tail.

## Dual Time Stepping (Jameson 1991)

Introducing superscripts  $n$  to denote the time level, the second order backward difference formula (BDF2) for time integration is

$$\frac{3V}{2\Delta t} \mathbf{w}^{n+1} - \frac{2V}{\Delta t} \mathbf{w}^n + \frac{V}{2\Delta t} \mathbf{w}^{n-1} + R(\mathbf{w}^{n+1}) = 0 \quad (2)$$

In the dual time stepping scheme this equation is solved by marching the equation

$$\frac{d\mathbf{w}}{d\tau} + R^*(\mathbf{w}) = 0 \quad (3)$$

to a steady state, where the modified residual is

$$R^*(\mathbf{w}) = R(\mathbf{w}) + \frac{3V}{2\Delta t} \mathbf{w} - \frac{2V}{\Delta t} \mathbf{w}^n - \frac{V}{2\Delta t} \mathbf{w}^{n-1} \quad (4)$$



## Implicit Runge-Kutta Schemes

The dual time stepping approach has been quite widely adopted, particularly in conjunction with the BDF2 scheme, which is both A and L-stable. Dahlquist has proved that A-stable linear multi-step schemes are at most second order accurate [Dah63]. In the works of Butcher and other specialists in the numerical solution of ordinary differential equations it has been shown that it is possible to design A and L-stable implicit Runge-Kutta schemes which yield higher order accuracy [But87, But03, But64].

Recently there has been considerable interest in whether implicit Runge-Kutta schemes can achieve better accuracy for a given computational cost than the backwards difference formulas. Most of the studies to date have focused on diagonal implicit Runge-Kutta (DIRK) schemes, sometimes called semi-implicit schemes, in which the stages may be solved successively. These schemes, however, need a large number of stages. For example, the scheme of Kennedy and Carpenter uses one explicit and five implicit stages to attain fourth order accuracy [BCVK02].

## Two Stage Fourth Order Gauss Scheme

For equation 1, the two stage Gauss scheme takes the form

$$\begin{aligned}
 \xi_1 &= \mathbf{w}^n - \frac{\Delta t}{V} (a_{11}R(\xi_1) + a_{12}R(\xi_2)) \\
 \xi_2 &= \mathbf{w}^n - \frac{\Delta t}{V} t (a_{21}R(\xi_1) + a_{22}R(\xi_2)) \\
 \mathbf{w}^{n+1} &= \mathbf{w}^n - \frac{\Delta t}{2V} (R(\xi_1) + R(\xi_2))
 \end{aligned} \tag{5}$$

where the matrix  $A$  of coefficients is

$$A = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \end{bmatrix} \tag{6}$$

and the stage values correspond to Gauss integration points inside the time step with the values  $\left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right) \Delta t$  and  $\left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right) \Delta t$ .

## Three Stage Sixth Order Gauss Scheme

The three stage Gauss scheme takes the form

$$\begin{aligned}
 \xi_1 &= \mathbf{w}^n - \frac{\Delta t}{V} (a_{11}R(\xi_1) + a_{12}R(\xi_2) + a_{13}R(\xi_3)) \\
 \xi_2 &= \mathbf{w}^n - \frac{\Delta t}{V} (a_{21}R(\xi_1) + a_{22}R(\xi_2) + a_{23}R(\xi_3)) \\
 \xi_3 &= \mathbf{w}^n - \frac{\Delta t}{V} (a_{31}R(\xi_1) + a_{32}R(\xi_2) + a_{33}R(\xi_3)) \\
 \mathbf{w}^{n+1} &= \mathbf{w}^n - \frac{\Delta t}{18V} (5R(\xi_1) + 8R(\xi_2) + 5R(\xi_3))
 \end{aligned} \tag{7}$$

where the matrix  $A$  of coefficients is

$$A = \begin{bmatrix} \frac{5}{36} & \frac{2}{9} - \frac{\sqrt{15}}{15} & \frac{5}{36} - \frac{\sqrt{15}}{30} \\ \frac{5}{36} + \frac{\sqrt{15}}{30} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{24} \\ \frac{5}{36} + \frac{\sqrt{15}}{30} & \frac{2}{9} + \frac{\sqrt{15}}{15} & \frac{5}{36} \end{bmatrix} \tag{8}$$

and the stage values correspond to the intermediate times  $\left(\frac{1}{2} - \frac{\sqrt{15}}{10}\right) \Delta t$ ,  $\frac{1}{2} \Delta t$  and  $\left(\frac{1}{2} + \frac{\sqrt{15}}{10}\right) \Delta t$  within the time step.

## Two Stage Third Order Radau 2A Scheme

For the solution of equation 1, the two stage Radau 2A scheme takes the form

$$\begin{aligned}\xi_1 &= \mathbf{w}^n - \frac{\Delta t}{V} (a_{11}R(\xi_1) + a_{12}R(\xi_2)) \\ \xi_2 &= \mathbf{w}^n - \frac{\Delta t}{V} (a_{21}R(\xi_1) + a_{22}R(\xi_2)) \\ \mathbf{w}^{n+1} &= \xi_2\end{aligned}\tag{9}$$

where the matrix  $A$  of coefficients is

$$A = \begin{bmatrix} \frac{5}{12} & -\frac{1}{12} \\ \frac{3}{4} & \frac{1}{4} \end{bmatrix}$$

and the stage values correspond to Radau integration points at  $\frac{1}{3}\Delta t$  and  $\Delta t$ .

## Three Stage Fifth Order Radau 2A Scheme

The three stage Radau 2A scheme takes the form

$$\begin{aligned}
 \xi_1 &= \mathbf{w}^n - \frac{\Delta t}{V} (a_{11}R(\xi_1) + a_{12}R(\xi_2) + a_{13}R(\xi_3)) \\
 \xi_2 &= \mathbf{w}^n - \frac{\Delta t}{V} (a_{21}R(\xi_1) + a_{22}R(\xi_2) + a_{23}R(\xi_3)) \\
 \xi_3 &= \mathbf{w}^n - \frac{\Delta t}{V} (a_{31}R(\xi_1) + a_{32}R(\xi_2) + a_{33}R(\xi_3)) \\
 \mathbf{w}^{n+1} &= \xi_3
 \end{aligned} \tag{10}$$

where the matrix  $A$  of coefficients is

$$A = \begin{bmatrix} \frac{88-7\sqrt{6}}{360} & \frac{296-169\sqrt{6}}{1800} & \frac{-2+3\sqrt{6}}{225} \\ \frac{296+169\sqrt{6}}{1800} & \frac{88+7\sqrt{6}}{360} & \frac{-2-3\sqrt{6}}{225} \\ \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \end{bmatrix}$$

and the stage values correspond to the Radau integration points  $\frac{4-\sqrt{6}}{10} \Delta t$ ,  $\frac{4+\sqrt{6}}{10} \Delta t$  and  $\Delta t$ .

# Formulation

## Naive Application of Dual Time Stepping Schemes

In order to clarify the issues it is useful to consider first the application of the two stage Gauss scheme to the scalar equation

$$\frac{du}{dt} = au \quad (11)$$

where  $a$  is a complex coefficient lying in the left half plane. A naive application of dual time stepping would simply add derivatives in pseudo time to produce the scheme

$$\begin{aligned} \frac{d\xi_1}{d\tau} &= a(a_{11}\xi_1 + a_{12}\xi_2) + \frac{u^n - \xi_1}{\Delta t} \\ \frac{d\xi_2}{d\tau} &= a(a_{21}\xi_1 + a_{22}\xi_2) + \frac{u^n - \xi_2}{\Delta t} \end{aligned} \quad (12)$$

which may be written in vector form as

$$\frac{d\xi}{d\tau} = B\xi + c \quad (13)$$

where

$$B = \begin{bmatrix} a_{11}a - \frac{1}{\Delta t} & a_{12}a \\ a_{21}a & a_{22}a - \frac{1}{\Delta t} \end{bmatrix}, \quad c = \frac{1}{\Delta t} \begin{bmatrix} u^n \\ u^n \end{bmatrix}$$

## Naive Application of Dual Time Stepping Schemes

For equation (13) to converge to a steady state the eigenvalues of  $B$  should lie in the left half plane. These are the roots of

$$\det(\lambda I - B) = 0$$

or

$$\lambda^2 - \lambda \left( (a_{11} + a_{22})a - \frac{2}{\Delta t} \right) + a_{11}a_{22}a^2 - (a_{11} + a_{22})\frac{a}{\Delta t} + \frac{1}{\Delta t^2} - a_{12}a_{21}a^2 = 0$$

Substituting the coefficient values for the Gauss scheme given in equation (6), we find that

$$\lambda = \frac{1}{4}a - \frac{1}{\Delta t} \pm ia\sqrt{\frac{1}{48}}$$

Then if  $a = p + iq$

$$\lambda = \frac{1}{4}p \pm q\sqrt{\frac{1}{48}} - \frac{1}{\Delta t} + i \left( \frac{1}{4}q \pm p\sqrt{\frac{1}{48}} \right)$$

and for small  $\Delta t$  one root could have a positive real part even when  $a$  lies in the left plane.



## Preconditioned Dual Time-Stepping Scheme for Two Stage Schemes

In order to prevent this we can modify equation (12) by multiplying the right hand side by a preconditioning matrix. It is proposed here to take the inverse of the Runge-Kutta coefficient array  $A$  as the preconditioning matrix. Here

$$A^{-1} = \frac{1}{D} \begin{bmatrix} a_{22} & -a_{12} \\ a_{21} & a_{11} \end{bmatrix}$$

where the determinant of  $A$  is

$$D = a_{11}a_{22} - a_{12}a_{21}$$

Setting

$$r_1 = a(a_{11}\xi_1 + a_{12}\xi_2) + \frac{u^n - \xi_1}{\Delta t}$$

$$r_2 = a(a_{21}\xi_1 + a_{22}\xi_2) + \frac{u^n - \xi_2}{\Delta t}$$

the preconditioned dual time stepping scheme now takes the form

$$\begin{aligned} \frac{d\xi_1}{d\tau} &= (a_{22}r_1 - a_{12}r_2)D \\ &= a\xi_1 + \frac{a_{22}}{D\Delta t} (u^n - \xi_1) - \frac{a_{12}}{D\Delta t} (u^n - \xi_2) \\ \frac{d\xi_2}{d\tau} &= (a_{11}r_2 - a_{21}r_1)/D \\ &= a\xi_2 + \frac{a_{11}}{D\Delta t} (u^n - \xi_2) - \frac{a_{21}}{D\Delta t} (u^n - \xi_1) \end{aligned}$$

## Preconditioned Dual Time-Stepping Scheme for Two Stage Schemes

The preconditioned dual time stepping scheme may be written in the vector form (13) where now

$$B = \begin{bmatrix} a - \frac{a_{22}}{D\Delta t} & \frac{a_{12}}{D\Delta t} \\ \frac{a_{21}}{D\Delta t} & a - \frac{a_{11}}{D\Delta t} \end{bmatrix}, \quad c = \frac{1}{D\Delta t} \begin{bmatrix} (a_{22} - a_{12})u^n \\ (a_{11} - a - 21)u^n \end{bmatrix}$$

Now the dual time stepping scheme will reach a steady state if the roots of

$$\det(\lambda I - B) = 0$$

lie in the left half plane. Substituting the coefficients of  $B$  the roots satisfy

$$\lambda^2 - \lambda \left( 2a - \frac{a_{11} + a_{22}}{D\Delta t} \right) + a^2 - a \frac{a_{11} + a_{22}}{D\Delta t} + \frac{1}{D} \Delta t^2 = 0$$

and using the coefficient values of the Gauss scheme, we now find that

$$\lambda^2 - \lambda \left( 2a - \frac{6}{\Delta t} \right) + a^2 - \frac{6a}{\Delta t} + \frac{12}{\Delta t^2} = 0$$

yielding

$$\lambda = a - \frac{3}{\Delta t} \pm i \frac{\sqrt{3}}{\Delta t}$$

## Dual Time-Stepping Scheme for Two Stage IRK Schemes

Following this approach, the proposed dual time stepping scheme for the nonlinear equations (5) is

$$\begin{aligned}\mathbf{r}_1 &= \frac{V}{\Delta t}(\mathbf{w}^n - \boldsymbol{\xi}_1) - a_{11}R(\boldsymbol{\xi}_1) - a_{12}R(\boldsymbol{\xi}_2) \\ \mathbf{r}_2 &= \frac{V}{\Delta t}(\mathbf{w}^n - \boldsymbol{\xi}_2) - a_{21}R(\boldsymbol{\xi}_1) - a_{22}R(\boldsymbol{\xi}_2)\end{aligned}\tag{14}$$

and

$$\begin{aligned}\frac{d\boldsymbol{\xi}_1}{d\tau} &= (a_{22}\mathbf{r}_1 - a_{12}\mathbf{r}_2)/D \\ \frac{d\boldsymbol{\xi}_2}{d\tau} &= (a_{11}\mathbf{r}_2 - a_{21}\mathbf{r}_1)/D\end{aligned}\tag{15}$$

where  $D$  is the determinant of  $A$ .

## General Approach to Dual Time-Stepping Scheme for IRK Schemes

Using vector notation a naive application of dual time stepping yields the equations

$$\frac{d\xi}{d\tau} = aA\xi + \frac{1}{\Delta t} (w^n - \xi) \quad (16)$$

and the eigenvalues of the matrix

$$B = aA - \frac{1}{\Delta t} I \quad (17)$$

do not necessarily lie in the left half plane. Introducing  $A^{-1}$  as a preconditioning matrix the dual time stepping equations become

$$\frac{d\xi}{d\tau} = a\xi + \frac{1}{\Delta t} A^{-1} (w^n - \xi) \quad (18)$$

so we need the eigenvalues of

$$B = aI - \frac{1}{\Delta t} A^{-1} \quad (19)$$

to lie in the left half plane for all values of  $a$  in the left half plane. The eigenvalues of  $B$  are

$$a - \frac{1}{\Delta t} \frac{1}{\lambda_k}, \quad k = 1, 2, 3$$

where  $\lambda_k$  are the eigenvalues of  $A$ . Thus they will lie in the left half plane for all values of  $a$  in the left half plane if the eigenvalues of  $A$  lie in the right half plane.

## Characteristic Polynomials of the Two Stage Schemes

The characteristic polynomials of  $A$  for the two-stage Gauss and Radau 2A schemes are

$$\lambda^2 - \frac{1}{2}\lambda + \frac{1}{12} = 0$$

and

$$\lambda^2 - \frac{2}{3}\lambda + \frac{1}{6} = 0$$

with roots

$$\lambda = \frac{1}{4} \pm i\sqrt{\frac{1}{48}}$$

and

$$\lambda = \frac{1}{3} \pm i\sqrt{\frac{1}{18}}$$

respectively, which in both cases lie in the right half plane.

## Characteristic Polynomials of the Three Stage Schemes

The characteristic polynomials for the three stage Gauss and Radau 2A schemes are

$$\lambda^3 - \frac{1}{2}\lambda^2 + \frac{1}{10}\lambda - \frac{1}{120} = 0 \quad (20)$$

and

$$\lambda^3 - \frac{6}{10}\lambda^2 + \frac{3}{20}\lambda - \frac{1}{60} = 0. \quad (21)$$

Rather than calculating the roots directly, it is simpler to use the Routh-Hurwitz criterion which states that the roots of

$$a_3\lambda^3 + a_2\lambda^2 + a_1\lambda + a_0$$

lie in the left half plane if all the coefficients are positive and

$$a_2a_1 > a_3a_0.$$

The roots of  $A$  will lie in the right half plane if the roots of  $-A$  be in the left half plane. Here, the characteristic polynomials of  $-A$  for the two-three stage schemes are

$$\lambda^3 + \frac{1}{2}\lambda^2 + \frac{1}{10}\lambda + \frac{1}{120}$$

and

$$\lambda^3 + \frac{6}{10}\lambda^2 + \frac{3}{20}\lambda + \frac{1}{60}$$

and it is easily verified that the Routh-Hurwitz condition is satisfied in both cases.

## Dual Time Stepping Scheme for the Three Stage IRK Schemes

The proposed dual time stepping scheme for the three stage schemes is now

$$\mathbf{r}_1 = \frac{V}{\Delta t} (\mathbf{w}^n - \boldsymbol{\xi}_1) - a_{11}R(\boldsymbol{\xi}_1) - a_{12}R(\boldsymbol{\xi}_2) - a_{13}R(\boldsymbol{\xi}_3)$$

$$\mathbf{r}_2 = \frac{V}{\Delta t} (\mathbf{w}^n - \boldsymbol{\xi}_2) - a_{21}R(\boldsymbol{\xi}_1) - a_{22}R(\boldsymbol{\xi}_2) - a_{23}R(\boldsymbol{\xi}_3)$$

$$\mathbf{r}_3 = \frac{V}{\Delta t} (\mathbf{w}^n - \boldsymbol{\xi}_3) - a_{31}R(\boldsymbol{\xi}_1) - a_{32}R(\boldsymbol{\xi}_2) - a_{33}R(\boldsymbol{\xi}_3)$$

and

$$\frac{d\boldsymbol{\xi}_1}{d\tau} = d_{11}\mathbf{r}_1 + d_{12}\mathbf{r}_2 + d_{13}\mathbf{r}_3$$

$$\frac{d\boldsymbol{\xi}_2}{d\tau} = d_{21}\mathbf{r}_1 + d_{22}\mathbf{r}_2 + d_{23}\mathbf{r}_3$$

$$\frac{d\boldsymbol{\xi}_3}{d\tau} = d_{31}\mathbf{r}_1 + d_{32}\mathbf{r}_2 + d_{33}\mathbf{r}_3$$

where the coefficients  $d_{jk}$  are the entries of  $A^{-1}$ .

## Applications to the Unsteady Euler Equations

These schemes have been applied to solve the Euler equations for unsteady flow past a pitching airfoil with these implicit Runge-Kutta schemes. The spatial discretization uses the Jameson-Schmidt-Turkel (JST) scheme[JST81]. The dual time stepping equations (15) are solved by a three stage preconditioned Runge-Kutta scheme similar to that proposed by Rossow[Ros07] and Swanson et al [STR07]. Writing the dual time stepping equations as

$$\frac{d\xi}{d\tau} + R^*(\xi) = 0$$

the scheme takes the general form

$$\xi^{(1)} = \xi^{(0)} - \alpha_1 \Delta\tau P^{-1} R^* \left( \xi^{(0)} \right)$$

$$\xi^{(2)} = \xi^{(0)} - \alpha_2 \Delta\tau P^{-1} R^* \left( \xi^{(1)} \right)$$

$$\xi^{(3)} = \xi^{(0)} - \alpha_3 \Delta\tau P^{-1} R^* \left( \xi^{(4)} \right)$$

where

$$\alpha_1 = 0.15, \alpha_2 = 0.40, \alpha_3 = 1$$

and  $P^{-1}$  denotes a single sweep of an LUSGS scheme in each direction.



# Results

## Flow Past a Pitching Airfoil

The flow past a pitching airfoil has been used as a test case for the new dual time stepping implicit Runge-Kutta schemes. The selected case is the A GARD case CT-6. This is a pitching NACA 64A010 airfoil at a Mach number of 0.796. The airfoil is symmetric and the mean angle of attack is zero, leading to a flow in which shock waves appear alternately on the upper and lower surface. The pitching amplitude is  $\pm 1.01$  degrees, and the reduced frequency, defined as

$$k = \frac{\omega_{\text{chord}}}{2q_{\infty}}$$

where  $\omega$  is the pitching rate, has a value of 2.02. Calculations were performed on an O-mesh with  $160 \times 32$  cells (displayed in Figure 2), which has a very tight spacing at the trailing edge. An initial steady state was established using 50 multigrid cycles. These were sufficient to reduce the density residual to a value less than  $10^{-12}$ . Then 6 pitching cycles were calculated with the dual time stepping scheme. This is sufficient to reach an almost steady periodic state. The implicit time step was selected such that each pitching cycle was calculated with 18 steps, corresponding to a shift of 20 degrees in the phase angle per step.

# O-Mesh Used in Pitching Airfoil Calculations

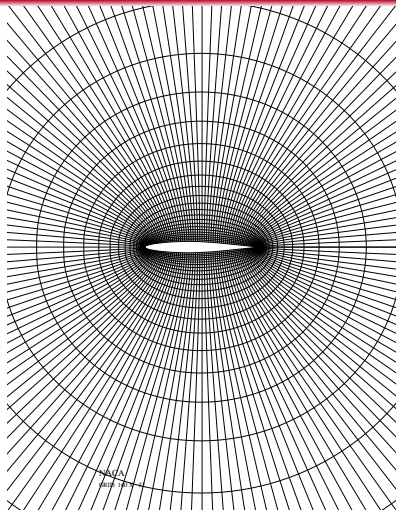


Figure 2: O-mesh used in pitching airfoil calculations

# Convergence History of the Inner Iterations of the Last Step

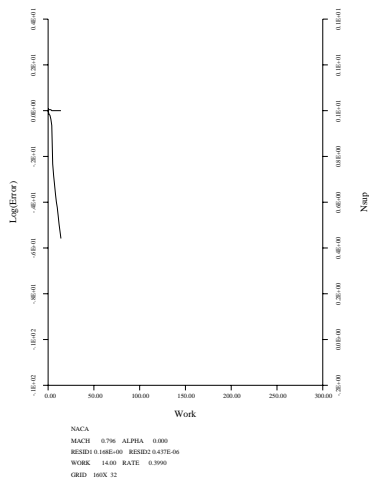


Figure 3: Convergence history of the inner iterations of the last step

# Snapshot of the Solution at Several Phase Angles During the Sixth Pitching Cycle

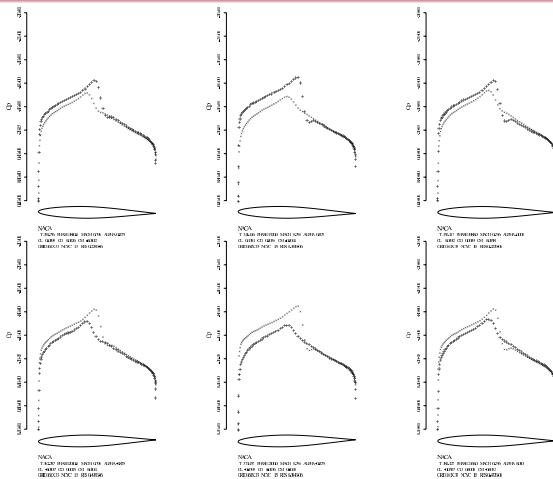


Figure 4: Snapshot of the solution at several phase angles during the sixth pitching cycle

# Lift coefficient $C_L$ versus angle of attack $\alpha$

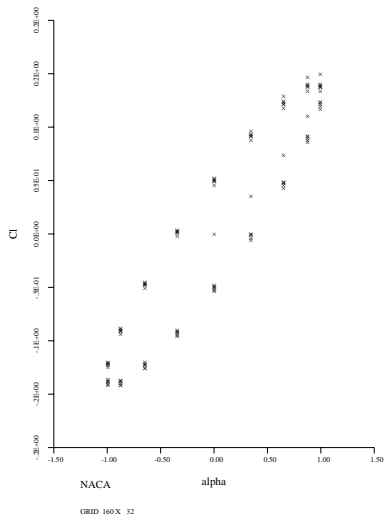


Figure 5: Lift coefficient  $C_L$  versus angle of attack  $\alpha$

# Conclusion

## Conclusion

Dual time stepping is a feasible approach for solving the coupled residual equations of a fully implicit Runge-Kutta schemes for unsteady flow simulations. The fourth and sixth order Gauss schemes appear to be competitive with alternative implicit schemes because they require only two and three stages respectively and they are A-stable although not L-stable. It seems, therefore, that they merit further study.



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