Multigrid Direct Numerical Simulation of the Whole Process of Flow Transition in 3-D Boundary Layers

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Abstract
A new technology was developed in this study which provides a successful numerical simulation of the whole process of flow transition in 3-D boundary layers, including linear growth, secondary instability, breakdown, and transition at relatively low CPU cost. Most other spatial numerical simulations require high CPU cost and blow up at the stage of flow breakdown. A fourth-order finite difference scheme on stretched and staggered grids, a fully implicit time-marching technique, a semi-coarsening multigrid based on the so-called approximate line-box relaxation, and a buffer domain for the outflow boundary conditions were all used for high-order accuracy, good stability, and fast convergence. A new fine-coarse-fine grid mapping technique was developed to keep the code running after the laminar flow breaks down. The computational results are in good agreement with linear stability theory, secondary instability theory, and some experiments. The cost for a typical case with $162 \times 34 \times 34$ grid is around 2 CRAY-YMP CPU hours for 10 T-S periods.

1 Introduction

The transition process from laminar to turbulent flow in a wall-bounded shear flow is still a challenging and unsolved problem. Natural transition is a multi-stage process (Narasimha, 1990) involving 2-D linear evolution, 3-D secondary instability, breakdown, and transition (Figure 1).

The linear stability equation was established by Orr (1907a, b) and Sommerfeld (1908), was solved by Tollmien (1931) and Schlichting (1932), and was experimentally confirmed by Schubauer and Skramstad (1948). The secondary instability was observed by Klebanoff, Tidstrom & Sargent (1962) for K-type fundamental transition, and was observed by Kachanov, Kozlov and Levchenko (1978) for subharmonic transition. The theoretical work was accomplished by Herbert (1983a & 1983b). There is really very little work, either theoretical or experimental, about the breakdown and transition zones which are the major parts of transition process.
The numerical study of transition is still quite limited due to the lack of computational resources. First, most numerical studies are temporal (Orszag & Kells, 1980; Wray & Hussaini, 1984; Kleiser & Laurien, 1985; Zang & Hussaini, 1986; Zang, Krist, Erlebader, & Hussaini, 1987). They can provide better resolution but lack physically realistic representation (Joslin et al. 1992).

Second, although there have been some spatial studies (Fasel, 1976; Fasel & Bestek, 1986; Fasel & Konzelmann, 1990; Spalart, 1989; Danabasoglu, Biringen, & Streett, 1991), the spatial direct numerical simulation (DNS) is still in its early age (Kleiser & Zang, 1991). Most of these can predict only the early stages of transition (pre-onset simulation) or fully developed turbulent flow without a transition process and require high CPU cost which is in the range of 100-1000 CRAY-YMP CPU hours.

In contrast, the current study has two advantages. First, it was successful in spatial DNS for the whole process of transition including linear evolution, secondary instability, breakdown, and transition to turbulence. Second, the current approach is more efficient. The spatial DNS was carried out on a rather coarse grid (16 × 34 × 34 for each T-S wavelength) at an acceptable CPU cost which is in the range of 2 - 10 CRAY-YMP hours.

Figure 1. Idealized sketch of transition process on a flat plate.
2 Governing Equation In General Coordinates

Let

\[ \begin{align*}
    x &= x(\xi, \eta, \zeta), \\
    y &= y(\xi, \eta, \zeta), \\
    z &= z(\xi, \eta, \zeta),
\end{align*} \]

the 3-D time-dependent incompressible Navier-Stokes equations can then be written as

\[ \begin{align*}
    U &= \frac{1}{J}(u\xi_x + v\xi_y + w\xi_z), \\
    V &= \frac{1}{J}(u\eta_x + v\eta_y + w\eta_z), \\
    W &= \frac{1}{J}(u\zeta_x + v\zeta_y + w\zeta_z),
\end{align*} \]  

(1) \hspace{1cm} (2) \hspace{1cm} (3)

and

\[ \begin{align*}
    \frac{\partial u}{\partial t} + J&\left(\frac{\partial U u}{\partial \xi} + \frac{\partial V u}{\partial \eta} + \frac{\partial W u}{\partial \zeta}\right) + (\xi \frac{\partial}{\partial \xi} + \eta \frac{\partial}{\partial \eta} + \zeta \frac{\partial}{\partial \zeta})P - \frac{1}{Re} \Delta_1 u &= 0, \\
    \frac{\partial v}{\partial t} + J&\left(\frac{\partial U v}{\partial \xi} + \frac{\partial V v}{\partial \eta} + \frac{\partial W v}{\partial \zeta}\right) + (\xi \frac{\partial}{\partial \xi} + \eta \frac{\partial}{\partial \eta} + \zeta \frac{\partial}{\partial \zeta})P - \frac{1}{Re} \Delta_1 v &= 0, \\
    \frac{\partial w}{\partial t} + J&\left(\frac{\partial U w}{\partial \xi} + \frac{\partial V w}{\partial \eta} + \frac{\partial W w}{\partial \zeta}\right) + (\xi \frac{\partial}{\partial \xi} + \eta \frac{\partial}{\partial \eta} + \zeta \frac{\partial}{\partial \zeta})P - \frac{1}{Re} \Delta_1 w &= 0,
\end{align*} \]  

(4) \hspace{1cm} (5) \hspace{1cm} (6)

\[ \begin{align*}
    \frac{\partial U}{\partial \xi} + \frac{\partial V}{\partial \eta} + \frac{\partial W}{\partial \zeta} &= 0, \\
    \frac{\partial^2 U}{\partial \xi^2} + \frac{\partial^2 V}{\partial \eta^2} + \frac{\partial^2 W}{\partial \zeta^2} &= 0.
\end{align*} \]  

(7)

where\( u, v, w \) are velocity components,\( U, V, W \) are contravariant velocity components, \( P \) is pressure, \( Re \) is the Reynolds number based on the free stream velocity \( U_\infty \), the viscosity parameter \( \nu \) and some reference length, for example, \( \delta_0^* \) which is the displacement thickness of boundary layer at inflow,

\[ Re = \frac{U_\infty \delta_0^*}{\nu}, \]

and \( \Delta_1 \) is the physical Laplacian operator transferred to the computational \((\xi, \eta, \zeta)\) space:

\[ \Delta_1 = (\xi_x^2 + \xi_y^2 + \xi_z^2) \frac{\partial^2}{\partial \xi^2} + (\eta_x^2 + \eta_y^2 + \eta_z^2) \frac{\partial^2}{\partial \eta^2} + (\zeta_x^2 + \zeta_y^2 + \zeta_z^2) \frac{\partial^2}{\partial \zeta^2} + 2(\xi_x \eta_x + \xi_y \eta_y + \xi_z \eta_z) \frac{\partial^2}{\partial \xi \partial \eta} + 2(\eta_x \zeta_x + \eta_y \zeta_y + \eta_z \zeta_z) \frac{\partial^2}{\partial \eta \partial \zeta} + (\xi_x + \eta_x + \zeta_x) \frac{\partial}{\partial \xi} + (\eta_x + \eta_y + \zeta_y) \frac{\partial}{\partial \eta} + (\zeta_x + \zeta_y + \zeta_z) \frac{\partial}{\partial \zeta}. \]  

(8)

Here, we have 7 equations for 7 unknowns, \( u, v, w, P, U, V, \) and \( W \).

The perturbation equations are obtained by decomposing the total flow into steady base flow and a perturbation. Using subscript 0 denote the base flow variables, and let

\[ \begin{align*}
    \vec{u}(x, y, z, t) &\rightarrow \vec{u}_0(x, y, z) + \vec{u}(x, y, z, t), \\
    \vec{V}(x, y, z, t) &\rightarrow \vec{V}_0(x, y, z) + \vec{V}(x, y, z, t), \\
    P(x, y, z, t) &\rightarrow P_0(x, y, z) + P(x, y, z, t),
\end{align*} \]  

(9)
where \( \vec{v} = (u, v, w) \), \( \vec{V} = (U, V, W) \), and noting the base flow itself also satisfies the Navier-Stokes equations, we obtain the governing system for the perturbations:

\[
\frac{\partial u}{\partial t} + J\left( \frac{\partial [u(U + U_0) + u_0U]}{\partial \xi} + \frac{\partial [u(V + V_0) + u_0V]}{\partial \eta} + \frac{\partial [u(W + W_0) + u_0W]}{\partial \zeta} \right) + \left( \xi \frac{\partial}{\partial \xi} + \eta \frac{\partial}{\partial \eta} + \zeta \frac{\partial}{\partial \zeta} \right) P - \frac{1}{Re} \Delta_1 u = 0, \tag{10}
\]

\[
\frac{\partial v}{\partial t} + J\left( \frac{\partial [v(U + U_0) + v_0U]}{\partial \xi} + \frac{\partial [v(V + V_0) + v_0V]}{\partial \eta} + \frac{\partial [v(W + W_0) + v_0W]}{\partial \zeta} \right) + \left( \xi \frac{\partial}{\partial \xi} + \eta \frac{\partial}{\partial \eta} + \zeta \frac{\partial}{\partial \zeta} \right) P - \frac{1}{Re} \Delta_1 v = 0, \tag{11}
\]

\[
\frac{\partial w}{\partial t} + J\left( \frac{\partial [w(U + U_0) + w_0U]}{\partial \xi} + \frac{\partial [w(V + V_0) + w_0V]}{\partial \eta} + \frac{\partial [w(W + W_0) + w_0W]}{\partial \zeta} \right) + \left( \xi \frac{\partial}{\partial \xi} + \eta \frac{\partial}{\partial \eta} + \zeta \frac{\partial}{\partial \zeta} \right) P - \frac{1}{Re} \Delta_1 w = 0, \tag{12}
\]

\[
\frac{\partial U}{\partial \xi} + \frac{\partial V}{\partial \eta} + \frac{\partial W}{\partial \zeta} = 0. \tag{13}
\]

Combined with (1)-(3), this system also has 7 equations and 7 unknowns for the perturbations. We perform the solving process as follows:

1. Perform the surface and grid generation processes to obtain the required Jacobian coefficients.
2. Solve system (1) – (7) to obtain the base flow solution. For a flat plate, we use the Blasius similarity solution for the base flow.
3. Solve system (1) – (3) and (10) – (13) to obtain the perturbation solution based on the above base flow.

3 Boundary Conditions

Benney-Lin type disturbances are imposed at the inflow boundary in this study:

\[
u(0, y, z, t) = \varepsilon_{2d} \text{Rea}\{\phi_{u2d} e^{-i\omega t}\} + \varepsilon_{3d+} \text{Rea}\{\phi_{u3d+} e^{i(\beta z - \omega t)}\} + \varepsilon_{3d-} \text{Rea}\{\phi_{u3d-} e^{i(-\beta z - \omega t)}\},
\]

\[
v\left(-\frac{\Delta z}{2}, y, z, t\right) = \varepsilon_{2d} \text{Rea}\{\phi_{v2d} e^{(-\alpha \frac{\Delta z}{2} - \omega t)}\} + \varepsilon_{3d+} \text{Rea}\{\phi_{v3d+} e^{(-\alpha \frac{\Delta z}{2} + \beta z - \omega t)}\} + \varepsilon_{3d-} \text{Rea}\{\phi_{v3d-} e^{(-\alpha \frac{\Delta z}{2} - \beta z - \omega t)}\},
\]

\[
w\left(-\frac{\Delta z}{2}, y, z, t\right) = \varepsilon_{3d+} \text{Rea}\{\phi_{w3d+} e^{(-\alpha \frac{\Delta z}{2} + \beta z - \omega t)}\} + \varepsilon_{3d-} \text{Rea}\{\phi_{w3d-} e^{(-\alpha \frac{\Delta z}{2} - \beta z - \omega t)}\}, \tag{14}
\]

where \( \omega \) is the real frequency of the disturbance, \( \beta \) is a real constant that represents the spanwise wavenumber, and \( \alpha = \alpha_R + i\alpha_I \) is the streamwise complex wavenumber obtained from linear stability theory. \( \phi_u, \phi_v, \phi_w \) are eigenfunctions for the Orr-Sommerfeld equation.
A no slip boundary condition is applied at the solid wall. According to the linear stability theory, the disturbances vanish at infinity, so we obtain the boundary conditions at far field given by
\begin{align}
u(x, y \to \infty, z, t) &= 0, \\
v(x, y \to \infty, z, t) &= 0, \\
w(x, y \to \infty, z, t) &= 0. \quad (15)
\end{align}
Also, no pressure condition is needed at the inflow, solid wall, or far field since a staggered grid is used.

4 Outflow Boundary Treatment

Outflow boundary conditions have been the focus of study for the spatial simulation of flow transition by many researchers. For simplicity, we only describe the idea for a 2-D flat plate. The technique for the 3-D problem is the same.

Taking the advantage of the staggered grid, we can obtain a fairly effective approach. First, a buffer domain technique developed by Streett & Macaraeg (1989) is applied to our problem. Thus, a buffer domain is appended to the end of the original outflow boundary to smear all possible reflections from the buffered outflow boundary (see Figure 2). The problem is, in general, that the conventional buffer domain is too long (usually four to eight T-S wavelengths), which greatly increases computation cost. Our goal is to maintain the accuracy in the original computational domain, and to eliminate all the possible reflection waves in a very short buffer domain. To realize the above goal, the governing equations in the buffer domain should be parabolicized to allow only strictly outgoing waves. Thus, a first buffer function \( b(\xi) \) is introduced here and applied to the streamwise viscous terms:
\begin{align}
\frac{\partial^2 U}{\partial \xi^2} \to b(\xi) \frac{\partial^2 U}{\partial \xi^2}, \quad \frac{\partial^2 V}{\partial \xi^2} \to b(\xi) \frac{\partial^2 V}{\partial \xi^2}. \quad (16)
\end{align}
b(\xi) is a monotonically decreasing function that changes from 1 to 0 so that the upstream effects of the streamwise viscous terms will gradually disappear in the buffer domain. The essential feature here is that all damping mode disturbances at the buffered outflow boundary become zero. To understand this, we rewrite the first equation of (16) as
\begin{align}
b(\xi) \frac{\partial^2 U}{\partial \xi^2} \to \frac{\partial^2 U}{\partial \left[ \frac{\xi}{\sqrt{b(\xi)}} \right]^2}, \quad (17)
\end{align}
Since \( b(\xi) \to 0 \) at the buffered outflow boundary, and accordingly \( \sqrt{b(\xi)} \to \infty \), then, we can also consider that the buffered outflow boundary is compressed from \( \xi = \infty \) by the function \( \sqrt{b(\xi)} \). Now clearly, if the disturbances are stable (damping modes), they will vanish at \( \xi = \infty \). To treat unstable (growing) modes, we need a second buffer function \( b_{Re}(\xi) \) that reduces the Reynolds number in the buffer domain gradually to less than the critical (or subcritical) Reynolds number and makes all the perturbation modes become damping

\[
\frac{1}{Re} \to \frac{b_{Re}(\xi)}{Re}.
\]

Thus, the new modified governing equations in the computational \((\xi, \eta)\) plane become:

\[
\frac{\partial U}{\partial t} + \frac{1}{y_\eta} \frac{\partial(UU + 2UU_0)}{\partial \xi} + \frac{\partial}{\partial \eta} \left( \frac{U_0V + UV_0 + UV}{y_\eta} \right) - \frac{b_{Re}}{Re_0} \left( b \cdot \frac{\partial^2 U}{\partial \xi^2} + \frac{1}{y_\eta} \frac{\partial^2 U}{\partial \eta^2} \left( \frac{U}{y_\eta} \right) + y_\eta \eta \eta \frac{\partial}{\partial \eta} \left( \frac{U}{y_\eta} \right) \right) = 0,
\]

\[
\frac{\partial V}{\partial t} + \frac{\partial(U_0V + UV_0 + UV)}{\partial \xi} + \frac{\partial}{\partial \eta} \left( 2V_0V + VV \right) - \frac{b_{Re}}{Re_0} \left( b \cdot \frac{\partial^2 V}{\partial \xi^2} + \frac{1}{y_\eta} \frac{\partial^2 V}{\partial \eta^2} + y_\eta \eta \eta \frac{\partial}{\partial \eta} \left( \frac{V}{y_\eta} \right) + \frac{\partial P}{\partial \eta} \right) = 0,
\]

\[
\frac{\partial U}{\partial \xi} + \frac{\partial V}{\partial \eta} = 0.
\]

The buffer functions are chosen as follows:

\[
b(\xi) = \begin{cases} \tanh \left( \frac{L_{\text{total}} - \xi}{L_{\text{original}}} \right) & \text{for } L_{\text{original}} \leq \xi \leq L_{\text{total}}, \\
1 & \text{for } 0 \leq \xi \leq L_{\text{original}}.\end{cases}
\]

\[
b_{Re}(\xi) = \begin{cases} (cL_{\text{original}})^2 + 1 & \text{for } L_{\text{original}} \leq \xi \leq L_{\text{total}}, \\
1 & \text{for } 0 \leq \xi \leq L_{\text{original}}.\end{cases}
\]

It is clear that the first function decreases from one to zero very rapidly as one moves from the original outflow boundary to the buffered outflow boundary. The second function increasing from 1 to \( c + 1 \) is a quadratic function that is continuously differentiable at the original outflow boundary. Note that the total effect of these buffer functions is that, toward the buffered outflow boundary:

- the momentum equations become increasingly convection dominated in the \( \xi \)-direction, while the equations generally become parabolic; and
- the momentum equations become highly diffusion dominated in the \( \eta \)-direction.

This treatment makes the outgoing waves propagate forward without reflection in the \( \xi \)-direction, and any oscillation in the \( \eta \)-direction will be effectively smeared in the buffer domain.
Finally, we need to specify the buffered outflow boundary conditions under these modified governing equations. The parabolic character of the above equations requires only two boundary conditions. As mentioned before, we have the disturbances tending to zero at the buffered outflow boundary (which is actually located at $\xi = \infty$), so one condition is

$$P = 0. \quad (23)$$

This is a very important condition since the elliptic character of pressure has not been modified in our new governing equation. Any improper condition for $P$ may cause trouble. For the second condition, we use the traditional extrapolation method for $V$, i.e.,

$$\frac{\partial^2 V}{\partial \xi^2} = 0. \quad (24)$$

Though this condition may not be so accurate, accuracy of solutions in the buffer domain is not so important, and the main concern is that there must be no reflection wave traveling back to the original computational domain.

Referring to Figure 3, condition (23) is imposed directly on $P$ by defining

$$P_C = 0. \quad (25)$$

This is an implicit condition. With it, the discrete continuity equation associated with $P_C$ is then used to define $U$ at the buffered boundary:

$$U_E = U_C - \frac{V_N - V_C}{\Delta \eta} \Delta \xi. \quad (26)$$

Condition (24) is imposed by determining $V$ at ghost points just outside the boundary:

$$V_E = 2V_C - V_W. \quad (27)$$

Note that the above treatment is only suitable for the perturbation equations.
5 Simplification

In this study, we still use rectangular but stretched grids obtained by a special but relatively simple mapping (Figure 4):

\[ z = \xi, \]
\[ y = y(\eta), \]
\[ z = \zeta. \tag{28} \]

This yields

\[ J = \eta_y, \]
\[ \xi_\eta = \zeta_\eta = 1, \]
\[ \xi_y = \zeta_y = \eta_z = \zeta_z = \zeta_y = 0. \tag{29} \]

For our numerical simulation, we choose the transformation function

\[ y(\eta) = \frac{y_{\max} \sigma \eta}{\eta_{\max} \sigma + y_{\max} (\eta_{\max} - \eta)}, \tag{30} \]

where \( y_{\max} \) is the height of the computational domain in the physical coordinates \( y \), \( \eta_{\max} \) is the height of the computational domain in the computational coordinate \( \eta \), and \( \sigma \) is a constant which can be used to adjust the concentration of grid points. This yields an inverse map

\[ \eta(y) = \frac{\eta_{\max} y_{\max} \sigma (\eta + y)}{y_{\max} (\sigma + y)}. \tag{31} \]

We can then obtain

\[ y_\eta = \frac{\eta_{\max} y_{\max} \sigma (\eta + y)}{[\eta_{\max} \sigma + y_{\max} (\eta_{\max} - \eta)]^2}, \tag{32} \]
\[ \eta_{\eta\eta} = -\frac{2 \eta_{\max} \sigma (\eta + y)}{y_{\max} (\sigma + y)^2}. \tag{33} \]

![Figure 4. y-direction stretched grid.](image)

Under the above mapping, the governing equations can be simplified:

\[ \frac{\partial u}{\partial t} + \eta_v \left( \frac{\partial [u(U + U_0) + u_0 U]}{\partial \xi} + \frac{\partial [u(V + V_0) + u_0 V]}{\partial \eta} + \frac{\partial [uW + u_0 W]}{\partial \zeta} \right) + \frac{\partial P}{\partial \xi} - \frac{1}{Re} \Delta_1 u = 0, \tag{34} \]
\[ \frac{\partial v}{\partial t} + \eta_v \left( \frac{\partial [v(U + U_0) + v_0 U]}{\partial \xi} + \frac{\partial [v(V + V_0) + v_0 V]}{\partial \eta} + \frac{\partial [vW + v_0 W]}{\partial \zeta} \right) + \eta_y \frac{\partial P}{\partial \eta} - \frac{1}{Re} \Delta_1 v = 0, \tag{35} \]
\[
\frac{\partial w}{\partial t} + \eta_y \left( \frac{\partial w(U + U_0) + w_0 U}{\partial \xi} + \frac{\partial [w(V + V_0) + w_0 V]}{\partial \eta} + \frac{\partial [wW + w_0 W]}{\partial \zeta} \right) + \frac{\partial P}{\partial \zeta} - \frac{1}{Re} \Delta_1 w = 0, \tag{36}
\]
\[
\frac{\partial U}{\partial \xi} + \frac{\partial V}{\partial \eta} + \frac{\partial W}{\partial \zeta} = 0, \tag{37}
\]
\[
U = \frac{u}{\eta_y}, \tag{38}
\]
\[
W = \frac{w}{\eta_y}, \tag{39}
\]
\[
V = v, \tag{40}
\]

where \(u, v, w, P, U, V, W\) are all fluctuating parts of the corresponding variables, and \(w_0, v_0, w_0, U_0, V_0, W_0\) represent the base flow (Blasius solution for the flat plate). The transferred Laplacian operator in the computational space is simplified as

\[
\Delta_1 = \frac{\partial^2}{\partial \xi^2} + \eta_y \frac{\partial^2}{\partial \eta^2} + \eta_y \frac{\partial^2}{\partial \zeta^2}, \tag{41}
\]

6 Discretization

We use a uniform staggered grid for our problem in the computational \((\xi, \eta, \zeta)\) space (Figure 5). Letting \(\phi\) denote a generic function, the second-order backward Euler difference in time direction can be written as

\[
\frac{\partial \phi}{\partial t} \sim \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t}, \tag{42}
\]

and the fourth-order central difference in space can be written as

\[
\frac{\partial \phi}{\partial \xi} (\xi) \sim -\phi(\xi + 2\Delta \xi) + 8\phi(\xi + \Delta \xi) - 8\phi(\xi - \Delta \xi) + \phi(\xi - 2\Delta \xi), \tag{43}
\]
\[
\frac{\partial^2 \phi}{\partial \xi^2} (\xi) \sim -\phi(\xi + 2\Delta \xi) + 16\phi(\xi + 2\Delta \xi) - 30\phi(\xi + \Delta \xi) + 16\phi(\xi - \Delta \xi) - \phi(\xi - 2\Delta \xi), \tag{44}
\]
\[
\frac{\partial \phi}{\partial \xi} (\xi + \frac{1}{2} \Delta \xi) \sim -\phi(\xi + 2\Delta \xi) + 27\phi(\xi + \Delta \xi) - 27\phi(\xi) + \phi(\xi - \Delta \xi), \tag{45}
\]
Figure 5. Staggered grid structure in the computational ($\xi, \eta, \zeta$) space.

In the computational ($\xi, \eta, \zeta$) space, the grids are uniform. Suppose $u, v, w$ and $U, V, W$ are defined in terms of a staggered grid in the computational space (see Figure 5). Here, the values of $P$ are associated with its cell centers, $u$ and $U$ with centers of the cell surfaces parallel to the ($\eta, \zeta$) plane, $v$ and $V$ with centers of the cell surfaces parallel to the ($\xi, \zeta$) plane, and $w$ and $W$ with centers of the cell surfaces parallel to the ($\xi, \eta$) plane.

Second-order backward Euler differences are used in the time direction, and fourth-order central differences are used in space. We can write the discretized governing equations symbolically as follows (Figure 6):

\begin{align}
A_{EE} u_{EE} + A_{EU} E + A_{uw} w + A_{WW} v_{WW} + A_{NN} u_{NN} + A_{NN} u_{N} & + \\
A_{US} + A_{SS} u_{SS} + A_{PP} u_{PP} + A_{FP} + A_{BB} u_{BB} & = 0, \\
A_{uc} + D_{WW} P_{WW} + D_{WW} P_{w} + D_{BB} P_{B} - D_{C} P_{C} & = S_n, \quad (46) \\
B_{EE} v_{EE} + B_{EU} E + B_{wv} w + B_{WW} v_{WW} + B_{NN} v_{NN} + B_{NN} v_{N} & + \\
B_{VS} + B_{SS} v_{SS} + B_{PP} v_{PP} + B_{VP} + B_{BB} v_{BB} & = 0, \\
B_{vc} + E_{SS} P_{SS} + E_{SS} P_{s} + E_{N} P_{N} - E_{C} P_{C} & = S_n, \quad (47) \\
C_{EE} w_{EE} + C_{EW} E + C_{WW} w + C_{WW} w_{WW} + C_{NN} w_{NN} + C_{NN} w_{N} & + \\
C_{WS} + C_{SS} w_{SS} + C_{PP} w_{PP} + C_{WP} + C_{BB} w_{BB} & = 0, \\
C_{wc} + F_{SS} P_{SS} + F_{SS} P_{s} + F_{N} P_{N} - F_{C} P_{C} & = S_n, \quad (48) \\
D_{EE} U_{EE} + D_{EU} U + D_{wU} w + D_{WW} U_{WW} - D_{UC} U_{C} + D_{NN} U_{NN} & + \\
+ D_{V} V_{N} + D_{V} V_{s} - D_{V} V_{C} + D_{WW} P_{WW} + & = S_n, \quad (49)
\end{align}

As an illustration of the notation we use, relevant symbols for the discrete $\xi$-momentum equation are depicted in Figure 4. The coefficients and source term for the interior points of the discrete $\xi$-momentum equation (46)
associated with $u_C$ are given as follows:

\[
\begin{align*}
A_{EE} &= -\frac{1}{12Re\Delta \xi^2} + \frac{\eta_C}{12\Delta \xi} (U_{EE} + 2U_{os}), \\
A_E &= \frac{4}{3Re\Delta \xi^2} - \frac{2\eta_C}{3\Delta \xi} (U_E + 2U_o), \\
A_W &= \frac{4}{3Re\Delta \xi^2} + \frac{2\eta_C}{3\Delta \xi} (U_W + 2U_w), \\
A_{WW} &= -\frac{1}{12Re\Delta \xi^2} - \frac{2\eta_C}{12\Delta \xi} (U_{WW} + 2U_{oww}), \\
A_{NN} &= -\frac{\alpha_C}{12Re\Delta \eta^2} + \frac{\eta_C}{12\Delta \eta} (V_{nn} + V_{on}) - \frac{\gamma C}{12Re\Delta \eta}, \\
A_N &= \frac{4\alpha_C}{3Re\Delta \eta^2} - \frac{2\eta_C}{3\Delta \eta} (V_n + V_{on}) + \frac{2\gamma C}{3Re\Delta \eta}, \\
A_S &= \frac{4\alpha_C}{3Re\Delta \eta^2} + \frac{2\eta_C}{3\Delta \eta} (V_s + V_{os}) - \frac{2\gamma C}{3Re\Delta \eta}, \\
A_{SS} &= -\frac{\alpha_C}{12Re\Delta \eta^2} - \frac{\eta_C}{12\Delta \eta} (V_{ss} + V_{os}) + \frac{\gamma C}{12Re\Delta \eta}, \\
A_{PP} &= -\frac{1}{12Re\Delta \xi^2} + \frac{\eta_C}{12\Delta \xi} (W_{ff} + W_{of}), \\
A_{F} &= \frac{4}{3Re\Delta \xi^2} - \frac{2\eta_C}{3\Delta \xi} (W_f + W_o), \\
A_{B} &= \frac{4}{3Re\Delta \xi^2} + \frac{2\eta_C}{3\Delta \xi} (W_b + W_o), \\
A_{BB} &= -\frac{1}{12Re\Delta \xi^2} - \frac{\eta_C}{12\Delta \xi} (W_{bb} + W_{ob}), \\
A_{C} &= \frac{3}{2\Delta t} + \frac{5}{2Re} \left( \frac{1}{\Delta \xi^2} + \frac{\alpha_C}{\Delta \eta^2} + \frac{1}{\Delta \xi^2} \right), \\
D_E &= \frac{1}{24\Delta \xi}, \\
D_W &= D_C = \frac{27}{24\Delta \xi}, \\
D_{WW} &= -\frac{1}{24\Delta \xi}, \\
S_u &= -\frac{u_0^2 + u_0^{n-1}}{2\Delta t} + \eta_C \left( \frac{-u_{0NN}V_{nn} + 8u_{0N}V_n - 8u_{0S}V_s + u_{0SS}V_{ss}}{12\Delta \eta} \\
&\quad + \frac{-u_{0PP}W_{ff} + 8u_{0P}W_f - 8u_{0B}W_b + u_{0BB}W_{bb}}{12\Delta \xi} \right). \\
\end{align*}
\]

Here, superscripts $n$ and $n - 1$ are used to indicate values at previous time steps, and superscript $n + 1$, which indicates the current time step, is dropped for convenience. Lower case subscripts denote the approximate values of the $u$ and $w$ at points where the associated values of $u$ with capital subscript are located (Figure 6). Other symbols used in the above formulas are as follows:

\[
\alpha = \eta_y^2, \quad \gamma = \eta_{yy}.
\]
Figure 6. Neighbor points for $\xi$-momentum equation
($U$ are at the same points as $u$ and are not shown here).

All function values that are required at other than the canonical locations are obtained by fourth-order inter-
polations in the computational space. For example (see Figure 7),

$$V_c = (9(v_C + v_N + v_{NW} + v_W) - (v_{SWW} + v_{NNWW} + v_{SE} + v_{NNE}))/32,$$

Figure 7. Neighbor points for fourth-order approximation for $V_c$.

The coefficients for the $\eta-$ and $\zeta-$ momentum equations are defined in an analogous way, and the discrete
continuity equation is developed simply by applying the fourth-order central differences to each term.

7 Approximate Line-Box Relaxation (ALB)

7.1 2-D uniform grids

The basic approximate box relaxation (AB) approach is to relax by boxes instead of points. With a 2-D uniform
grid (Figure 8) as an example, we first describe the basic idea behind AB.
The generic form of the equations associated with a box for the 2-D uniform grids can be written as

\begin{align}
A_2^E u_E + A_2^W u_W + A_1^N u_N + A_1^S u_S - A_2^C u_C + \frac{P_W - P_C}{\Delta z} &= S_{uc}, \quad (53) \\
A_2^E u_{EE} + A_2^W u_C + A_1^N u_{NE} + A_1^S u_{SE} - A_2^C u_E + \frac{P_C - P_E}{\Delta z} &= S_{ue}, \quad (54) \\
B_2^E v_E + B_2^W v_W + B_1^N v_N + B_1^S v_S - B_2^C v_C + \frac{P_S - P_C}{\Delta y} &= S_{vc}, \quad (55) \\
B_2^N v_{NE} + B_2^W v_{NW} + B_1^N v_{NN} + B_1^S v_{SC} - B_2^C v_N + \frac{P_C - P_N}{\Delta y} &= S_{vn}, \quad (56) \\
\frac{u_E - u_C}{\Delta z} + \frac{v_N - v_C}{\Delta y} &= 0. \quad (57)
\end{align}

Here, the superscripts represent the point at which the discretization is centered. We proceed in the box-by-box process with a few global point Gauss-Seidel relaxation sweeps on the momentum equations, changing \( u \) and \( v \) and holding \( P \) fixed. This means that the four momentum equations (53)-(56) in the box phase are approximately satisfied. Now, proceeding by boxes in some order, we perform distributed relaxation of the form:

\begin{align}
&u_C \leftarrow u_C - \epsilon_1, \\
u_E \leftarrow u_E + \epsilon_2, \\
v_C \leftarrow v_C - \delta_1, \\
v_N \leftarrow v_N + \delta_2, \\
P_C \leftarrow P_C + \Delta P, \quad (58)
\end{align}

where the corrections are chosen to satisfy the discrete continuity equation and four discrete momentum equations associated with the box. Note that the old values of \( u, v, \) and \( P \) approximately satisfy the associated momentum equations, so we obtain the following system for the corrections, \( \epsilon_1, \epsilon_2, \delta_1, \delta_2, \) and \( \Delta P \):

\begin{align}
(A_2^E \epsilon_2 + A_2^C \epsilon_1) - \frac{\Delta P}{\Delta z} &= 0, \\
(A_1^E \epsilon_2 + A_1^C \epsilon_1) - \frac{\Delta P}{\Delta z} &= 0, \\
(B_2^C \delta_1 + B_2^E \delta_2) - \frac{\Delta P}{\Delta y} &= 0, \\
(B_1^C \delta_1 + B_1^E \delta_2) - \frac{\Delta P}{\Delta y} &= 0, \\
\frac{\epsilon_1 + \epsilon_2}{\Delta z} + \frac{\delta_1 + \delta_2}{\Delta y} &= S_m, \quad (59)
\end{align}

where

\[ S_m = -(\frac{u_E - u_C}{\Delta z} + \frac{v_N - v_C}{\Delta y}). \]
(59a) and (59b) yield
\[
\frac{\epsilon_1}{\epsilon_2} = \alpha \equiv \frac{A_C^E - A_W^E}{A_C^E - A_W^E},
\]
(59c) and (59d) yield
\[
\frac{\delta_1}{\delta_2} = \beta \equiv \frac{B_C^N - B_N^C}{B_C^E - B_N^C},
\]
and together we have
\[
\frac{\epsilon_1}{\delta_1} = \gamma \equiv \frac{B_C^E + \frac{F_C^E}{\alpha}}{A_C^E + \frac{A_C^E}{\alpha} \cdot \Delta y} \cdot \Delta x.
\]
Therefore, (59e) can be written as
\[
\frac{\epsilon_1}{\Delta x} + \frac{\delta_1}{\Delta y} = S_m,
\]
or
\[
\frac{\gamma(1 + \frac{1}{\alpha})\delta_1}{\Delta x} + \frac{(1 + \frac{1}{\beta})\delta_1}{\Delta y} = S_m.
\]
The correction are thus given by
\[
\delta_1 = \frac{S_m}{\gamma(1 + \frac{1}{\alpha}) + (1 + \frac{1}{\beta})},
\]
\[
\delta_2 = \frac{\delta_1}{\beta},
\]
\[
\epsilon_1 = \delta_1 \cdot \gamma,
\]
\[
\epsilon_2 = \frac{\epsilon_1}{\alpha},
\]
and
\[
\Delta P = (A_C^E \epsilon_1 + A_C^E \epsilon_2) \cdot \Delta x.
\]
To simplify this scheme, note that for the case \( \Delta t << 1 \), we have
\[
A_C^E \sim A_W^E, \quad B_C^E \sim B_N^C,
\]
\[
A_C^E >> A_W^E, \quad A_C^E >> A_W^E,
\]
\[
B_C^N >> B_N^C, \quad B_C^E >> B_N^C,
\]
so
\[
\alpha \approx 1, \quad \beta \approx 1, \quad \gamma \approx \frac{\Delta y}{\Delta x}.
\]
For most cases, we have
\[
A_C^E > A_W^E, \quad A_C^E > A_W^E,
\]
\[
B_C^N > B_N^C, \quad B_C^E > B_N^C,
\]
so \( \alpha, \beta \) and \( \gamma \) can be approximated in general by
\[
\alpha \sim \frac{A_C^E}{A_C^E} \sim 1, \quad \beta \sim \frac{B_C^E}{B_C^E} \sim 1, \quad \gamma \sim \frac{B_C^E}{A_C^E} \cdot \frac{\Delta y}{\Delta x}.
\]
It is these approximations and update formulas in (62) that we use in AB.
7.2 General coordinates

For general coordinates, the discrete momentum equations can still be written in the same generic form as that for Cartesian coordinates, but the continuity equation is changed to

\[
\frac{U_B - U_C}{\Delta \xi} + \frac{V_N - V_C}{\Delta \eta} = 0.
\]

(63)

The physical velocities \( u \) and \( v \) have the following relations with the contravariant velocities \( U \) and \( V \):

\[
U = au + bv, \\
V = cu + dv.
\]

This leads to the discrete continuity equation written as

\[
\frac{a_E u_E + b_E v_E - a_C u_C - b_C v_C}{\Delta \xi} + \frac{c_N u_N + d_N v_N - c_C u_C - d_C v_C}{\Delta \eta} = 0,
\]

where the superscript \( \sim \) represents a point that is not located at a canonical position and therefore requires interpolation. Assuming that

\[
(b_E \Delta u_E - b_C \Delta v_C) < (a_E \Delta u_E - a_C \Delta u_C),
\]

(64)

and

\[
(c_N \Delta u_N - c_C \Delta v_C) < (d_N \Delta v_N - d_C \Delta v_C),
\]

(65)

then the corresponding correction equation can be approximated by

\[
\frac{a_E \epsilon_2 + a_C \epsilon_1}{\Delta \xi} + \frac{d_N \delta_2 + d_C \delta_1}{\Delta \eta} = S_m.
\]

Note that the defining relations for \( \epsilon_1, \epsilon_2, \delta_1, \) and \( \delta_2 \) can be expressed in the same form as for Cartesian coordinates:

\[
\frac{\epsilon_1}{\epsilon_2} = a, \\
\frac{\delta_1}{\delta_2} = b, \\
\frac{\epsilon_1}{\delta_1} = c,
\]

and

\[
\delta_1 = \frac{S_m}{(\frac{\epsilon_1}{\epsilon_2} + a)\eta + (\frac{d_1}{\delta_1} + c)\eta},
\]

(66)

where \( a_E, a_C, d_N, d_C \) correspond to the mapping coefficients between \( u, v \) and \( U, V \).

7.3 Approximate line-box relaxation (ALB) for 3-D problems

ALB usually works well for 2-D problems, but frequently fails to provide fast convergence for 3-D problems. The basic idea of ALB is to satisfy the continuity equation for all boxes lying on one line simultaneously. Figure 9 gives the distribution of corrections in the \((\xi, \eta)\) plane for the ALB. This kind of relaxation is very useful when the grids are anisotropic. Assuming for simplicity that \( \alpha = \beta = 1 \), then according to Figure 9, ALB solving the discrete system (46)-(49) can be described as follows:

- Freezing \( P, U, V, W, \) and \( w \), perform line Gauss-Seidel relaxation on (46) over the entire computational domain to obtain a new \( u \).
- Freezing \( P, U, V, W, \) and \( w \), perform line Gauss-Seidel relaxation on (47) over the entire computational domain to obtain a new \( v \).
- Freezing \( P, U, V, W, \) and \( v \), perform line Gauss-Seidel relaxation on (48) over the entire computational domain to obtain a new \( w \).
- Use transformation (38)-(40) to obtain new \( U, V, W \).
For all $j = 2, 3, \cdots, n_j - 1$ at once: change $U_{i-\frac{1}{2}jk}, U_{i+\frac{1}{2}jk}, V_{ij-\frac{1}{2}jk}, W_{ij-\frac{1}{2}jk}$, and $W_{ij+\frac{3}{2}jk}$ to satisfy the associated continuity equations, then update $P_{ijk}$ so that the new $U, V, W$ and $P$ as well as the associated transferred $u, v, w$ satisfy the three momentum equations.

\begin{align*}
U_{i-\frac{1}{2}jk} + \Delta P_i &= 0, \\
V_{i \frac{3}{2}jk} + \delta_3 - \delta_6 &= 0, \\
U_{i+\frac{1}{2}jk} + \Delta P_i &= 0, \\
V_{i \frac{3}{2}jk} + \delta_4 - \delta_5 &= 0, \\
U_{i-\frac{1}{2}jk} + \Delta P_i &= 0, \\
V_{i \frac{3}{2}jk} + \delta_3 - \delta_4 &= 0, \\
U_{i+\frac{1}{2}jk} + \Delta P_i &= 0, \\
V_{i \frac{3}{2}jk} + \delta_2 - \delta_3 &= 0, \\
U_{i-\frac{1}{2}jk} + \Delta P_i &= 0, \\
V_{i \frac{3}{2}jk} + \delta_1 - \delta_2 &= 0.
\end{align*}

Figure 9. Distribution of corrections in the $(\xi, \eta)$ plane.

Since all of the $u, v, w$ have been previously relaxed, and the $U, V, W$ are updated, we assume that equations (46)-(48) hold exactly. Let $\epsilon, \delta, \sigma$ and $\Delta P$ represent the corrections for $U, V, W$ and $P$, respectively. Thus, for cube $ijk$ (see Figure 9), the correction equations corresponding to (46)-(49) are

\begin{align*}
(A_{ijk}^{\frac{1}{2}-jk} + A_{ijk}^{\frac{1}{2}jk}) \eta_{i\frac{1}{2}jk} + A_{ijk}^{\frac{1}{2}jk} \eta_{i\frac{1}{2}jk} &= 0, 
\tag{67} \\
B_{ij-\frac{1}{2}jk}^{\frac{1}{2}jk} (\delta_j - \delta_{j+1}) - B_{ij \frac{1}{2}jk}^{\frac{1}{2}jk} (\delta_{j+1} - \delta_j) - B_{ij \frac{1}{2}jk}^{\frac{1}{2}jk} \Delta P_j &= 0, 
\tag{68} \\
(C_{ijjk+\frac{1}{2}jk}^{\frac{1}{2}jk} + C_{ijjk-\frac{1}{2}jk}^{\frac{1}{2}jk} \eta_{i\frac{1}{2}jk}) \sigma_j - C_{ijjk-\frac{1}{2}jk}^{\frac{1}{2}jk} \Delta P_j &= 0, 
\tag{69} \\
(DU_{ijjk}^{\frac{1}{2}jk} + DU_{ijjk}^{\frac{1}{2}jk}, jk) \sigma_j + (DW_{ijjk}^{\frac{1}{2}jk} + DW_{ijjk}^{\frac{1}{2}jk}, jk) \sigma_j \\
+ DV_{ijjk}^{\frac{1}{2}jk} (\delta_j - \delta_{j+1}) - DV_{ijjk}^{\frac{1}{2}jk} (\delta_{j+1} - \delta_j) &= S_{mijk}, 
\tag{70}
\end{align*}

where the superscripts represent the point at which the discretization is centered. This system has $4(n_j - 2)$ equations for $4(n_j - 2)$ variables. Unfortunately, coupling between the correction variables makes the problem somewhat complicated. To develop a simpler approximate system, define

\begin{align*}
\omega_{ij} &= \frac{\epsilon_j}{\delta_j}, \\
\omega_{ij} &= \frac{\sigma_j}{\delta_j}.
\end{align*}
Then, equation (70) can be written in terms of the unknowns \( \delta_j \) only:

\[
((DU_{i+\frac{1}{2},j,k} + DU_{i-\frac{1}{2},j,k})ω_{ij} + (DV_{i,j+\frac{1}{2},k} + DV_{i,j-\frac{1}{2},k}) + (DW_{i,j,k+\frac{1}{2}} + DW_{i,j,k-\frac{1}{2}})ω_{ij})\delta_j \\
- D_{ij}^{jk} \delta_{j-1} - D_{ij}^{jk} \delta_{j+1} = S_{m_{ijk}}. \tag{71}
\]

Let

\[
a_j = (DU_{i+\frac{1}{2},j,k} + DU_{i-\frac{1}{2},j,k})ω_{ij} + (DV_{i,j+\frac{1}{2},k} + DV_{i,j-\frac{1}{2},k})
+ (DW_{i,j,k+\frac{1}{2}} + DW_{i,j,k-\frac{1}{2}})ω_{ij}, \tag{72}
\]

\[
b_j = -D_{ij}^{jk} \delta_j, \tag{73}
\]

\[
c_j = -D_{ij}^{jk} \delta_j, \tag{74}
\]

Then we obtain the tridiagonal system

\[
\begin{bmatrix}
  a_2 & b_2 & & & & \\
  c_3 & a_3 & b_3 & & & \\
  & & & \ddots & & \\
  & & & & & a_{n_j-2} & b_{n_j-2} \\
  & & & & c_{n_j-1} & a_{n_j-1} & b_{n_j-2} \\
  \vdots & \vdots & \ddots & \vdots & \ddots & \ddots & \ddots \\
  & & & & & c_{n_j-2} & a_{n_j-2} & b_{n_j-2} \\
  \end{bmatrix}
\begin{bmatrix}
  \delta_2 \\
  \delta_3 \\
  \vdots \\
  \vdots \\
  \vdots \\
  \delta_{n_j-2} \\
  \delta_{n_j-1} \\
  \end{bmatrix}
= 
\begin{bmatrix}
  S_{m_{i+2,k}} \\
  S_{m_{i+2,k}} \\
  \vdots \\
  \vdots \\
  \vdots \\
  S_{m_{i,n_j-2,k}} \\
  S_{m_{i,n_j-1,k}} \\
  \end{bmatrix}. \tag{75}
\]

Thus, \( \delta_j, j = 2, 3, \cdots, n_j - 1 \) can be determined very efficiently. The other velocity corrections are given by

\[
e_j = ω_{ij} \delta_j, \\
\sigma_j = ω_{ij} \delta_j, \\
j = 2, 3, \cdots, n_j - 1.
\]

The \( U, V, \) and \( W \) are then updated on all cells in the \( i, k, \eta \)-line as follows:

\[
U_{i+\frac{1}{2},j,k} \leftarrow U_{i+\frac{1}{2},j,k} + e_j, \\
U_{i-\frac{1}{2},j,k} \leftarrow U_{i-\frac{1}{2},j,k} - e_j, \\
W_{i,j,k+\frac{1}{2}} \leftarrow W_{i,j,k+\frac{1}{2}} + \sigma_j, \\
W_{i,j,k-\frac{1}{2}} \leftarrow W_{i,j,k-\frac{1}{2}} - \sigma_j, \\
j = 2, 3, \cdots, n_j - 1, \tag{76}
\]

\[
V_{i,j-\frac{1}{2},k} \leftarrow V_{i,j-\frac{1}{2},k} + \delta_{j-1} - \delta_j, \\
j = 3, 4, \cdots, n_j - 1. \tag{77}
\]

\( P \) is then updated via

\[
P_{ijk} \leftarrow P_{ijk} + ΔP_j, \\
j = 2, 3, \cdots, n_j - 1. \tag{78}
\]

8 Semi-Coarsening Multigrid

For the large-scale algebraic system of the 3-D flows that must be solved at each time step, the usual relaxation methods by themselves are much too slow. To obtain optimal efficiency, we use a multigrid scheme based on AB and ALB described in the previous section. For simplicity of discussion, we consider only the two-grid case.

We use a full approximation scheme (FAS) to accommodate nonlinearities. A two-level FAS algorithm for an equation of the form

\[
P^h q^h = f^h \tag{79}
\]
may be described loosely as follows:

i) relax on $L^h \phi^h = f^h$,
ii) solve $L^{2h} \phi^{2h} = L^{2h} I_h^{2h} \phi^h + \bar{I}_h^{2h}(f^h - L^h \phi^h)$,
iii) replace $\phi^h \leftarrow \phi^h + I_h^h(f_{2h} - \bar{I}_h^{2h}\phi^h)$.

The notation we have introduced includes the difference operators $L^h$ and $L^{2h}$, the restriction operators $I_h^h$ (for the approximation) and $\bar{I}_h^{2h}$ (for the residual), and the interpolation operator $I_h^h$.

A full-coarsening strategy is generally ineffective for problems that favor special coordinate directions (e.g., anisotropic problems). To overcome this limitation, we consider now a special combination of semi-coarsening and line-box relaxation. The basic idea is to use line-box relaxation in one direction (say the $y$-direction) and coarsening only in the other two directions ($x$- and $z$-directions). A two-level staggered grid projected in the $(z, y)$-plane and $(z, z)$-plane is given in Figure 10.

The full weighting restriction is still used here for transferring the residual from fine to coarse grids. The stencils can be expressed as follows:

$$
\begin{align*}
\bar{I}_h^h (R_u) & : \begin{bmatrix} 1 & 1 & 1 \\ 1/4 & 1/4 & 1/4 \\ 1/8 & 1/8 & 1/8 \end{bmatrix}, \\
\bar{I}_h^h (R_x) & : \begin{bmatrix} 1 & 1/4 \\ 1/4 & 1/4 \\ 1/8 & 1/8 \end{bmatrix}, \\
\bar{I}_h^h (R_\omega) & : \begin{bmatrix} 1 & 1/4 \\ 1/4 & 1/4 \\ 1/8 & 1/8 \end{bmatrix}, \\
\bar{I}_h^h (R_m) & : \begin{bmatrix} 1 & 1 \\ 1/4 & 1/4 \\ 1/8 & 1/8 \end{bmatrix}.
\end{align*}
$$

(80)

These stencils can be explained geometrically as shown in Figures 11-12.
Figure 10. Two-level staggered grid structure for $z-z$ direction semi-coarsening: 
(a) fine grid projection on $(z,y)$ plane, (b) coarse grid projection on $(z,y)$ plane, 
(c) fine and coarse grid projection on $(z,z)$ plane.

Figure 11. Full-weighting restriction for (a) $z$-momentum equation, (b) $z$-momentum equation.

Figure 12. Full-weighting restriction for $y$-momentum and continuity equations.

For the restriction of variables, bilinear interpolation is used. Its stencils are

$$
\tilde{R}_h^2(u) : \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, \\
\tilde{R}_h^2(v) : \begin{bmatrix} \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{bmatrix}, \\
\tilde{R}_h^2(w) : \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}, \\
\tilde{R}_h^2(P) : \begin{bmatrix} \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{bmatrix}.
$$

(81)

For semi-coarsening, the coarse to fine transfer operators are based on linear interpolation:

$$
\tilde{F}_h^2(\Delta u) : \begin{bmatrix} \frac{3}{8} \\ \frac{1}{4} \end{bmatrix} \text{ for } \Delta u^h_1 \text{ or } \begin{bmatrix} \frac{3}{8} \\ \frac{1}{4} \end{bmatrix} \text{ for } \Delta u^h_2,
$$
The meaning of the above stencils is shown in Figures 13-15.

\[ \bar{P}_h(\Delta v) : \begin{bmatrix} \frac{3}{16} & \frac{3}{16} \\ \frac{3}{16} & \frac{1}{16} \end{bmatrix}, \]

\[ \bar{P}_h(\Delta w) : \begin{bmatrix} 1 & 0 \\ \frac{1}{4} & \frac{1}{4} \end{bmatrix} \text{ for } \Delta w^h \text{ or } \begin{bmatrix} \frac{3}{16} & \frac{1}{16} \\ \frac{3}{16} & \frac{1}{16} \end{bmatrix} \text{ for } \Delta w^2, \]

\[ \bar{P}_h(\Delta P) : \begin{bmatrix} \frac{1}{16} & \frac{1}{16} \\ \frac{3}{16} & \frac{3}{16} \end{bmatrix}. \]

Figure 13. Bilinear interpolation for \( \Delta u \).

Figure 14. Bilinear interpolation for \( \Delta w \).

Figure 15. Bilinear interpolation for \( \Delta v \) and \( \Delta P \),

(\( \Delta P \) and \( \Delta v \) are not located in the same \((z, z)\) plane.)
9 Fine-Coarse-Fine Grid Mapping

The spatial DNS usually meets difficulties after the flow goes into the breakdown stage when the shear layer is developed and the vortex breaks down to small scale vortices. The numerical simulation will thus have a huge energy burst, and the disturbance velocity will be amplified by tens or hundreds of times somewhere inside the flow field. The code then blows up. Apparently, it is not the physical case, but is largely caused by that the grid we used is not fine enough to resolve the small eddies which play the role to generate dissipations. To keep the numerical simulation going, we developed a fine-coarse-fine grid mapping technique. To explain this technique, let us see what happens for a 1-D problem. We do the fine to coarse grid restriction and the coarse to fine grid interpolation at each time step:

\[
\begin{align*}
    u_c &= I_{kh}^{2h} u_f^{old} \\
    u_f^{new} &= I_{kh}^h u_c
\end{align*}
\]

Here, \(I_{kh}^{2h}\) is a linear restriction and \(I_{kh}^h\) is a linear interpolation.

[Diagram]

\(K < 1\) modes \hspace{1cm} \(K = 1\) modes

Figure 16. Fine-coarse-fine mapping.

Define \(L\) as a section which has five grid points on the fine grid, and (assume \(u_A \equiv 0\))

\[
\alpha = \frac{\int_0^L |u_f^{new}| dx}{\int_0^L |u_f^{old}| dx}
\]

as the amplification factor.

Assume we have different frequency modes, e.g.,

\[
\sin\left(\frac{2\pi}{L} z\right), \quad K = 1, \frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \ldots
\]

\((K > 1\) is not visible on this grid\), we can approximately get \(\alpha\) by numerical integration for different modes.

\[
\alpha = \frac{\left[\sin\left(\frac{2\pi}{L} \frac{1}{4}\right) + \frac{1}{2} \sin\left(\frac{2\pi}{L} \frac{1}{2}\right)\right]_2}{\left[\sin\left(\frac{2\pi}{L} \frac{1}{4}\right) + \frac{1}{2} \sin\left(\frac{2\pi}{L} \frac{1}{2}\right)\sin\left(\frac{2\pi}{L} \frac{5}{8}\right) + \frac{1}{2} \sin\left(\frac{2\pi}{L} \frac{3}{4}\right)\right]_4}
\]

\[
= \frac{2 \sin(K\pi) + \sin(2K\pi)}{\sin\left(\frac{K\pi}{2}\right) + \sin(K\pi) + \sin\left(\frac{3}{2}K\pi\right) + \frac{1}{2} \sin(2K\pi)}.
\]
when $K = 1$, $\alpha = 0$, when $K \to 0$, $\alpha \to 1$.

Figure 17 clearly shows that this kind of grid mapping, fine to coarse restriction and coarse to fine interpolation, significantly damps the highest frequency ($K = 1$), but has only a little effect on other modes ($K < 1$), and has almost no effect on low frequency modes ($K \to 0$).

The computational resources are still quite limited for DNS even if we use today's largest supercomputer. For certain grids, the highest frequency which can be well simulated is $K = 1$. This highest mode may generate higher frequencies which can not be simulated by current grids and may cause the computation to fail. This fine-coarse-fine grid mapping damps the $K = 1$ mode and protects other frequency modes. Of course, we do not want to eliminate the $K = 1$ mode, but to restrict its energy growth. The actual procedure of this technique is

1. $u_c = I_{h}^{2h}u_{f}^{old}$,
2. $u_{new}^{new} = (1 - \beta)u_{f}^{old} + \beta I_{h}^{2h}u_{c}$.

Here, we choose

$$\beta = \gamma \cdot (u^2 + v^2 + w^2),$$

which is proportional to the perturbation energy. Therefore, there is very little damping to $K = 1$ when the perturbation is very small. In this way, we successfully keep the code running to simulate the whole process of transition: linear evolution, secondary instability, breakdown, and transition. Note that the large eddies play a much more important role in flow transition than do small eddies which correspond to high frequency modes. We have to sacrifice these small eddies due to the lack of computer resources. But, the physics of transition and turbulence are still simulated quite well due to the accurate representation of lower frequency modes corresponding to large eddies.

10 Computational Results

10.1 Comparison with linear stability theory (LST)

To verify the accuracy of our approach, we compare our results with the linear theory by assuming a parallel steady base flow and imposing a small disturbance at inflow. The base flow is now $u_0(x, y) = u_0(x, y)$, $v_0(x, y) = 0$, where $u_0(x_0, y)$ is the Blasius similarity solution at inflow. Since it is easy for finite difference schemes to simulate the damping (stable) modes, we just test the growing (unstable) modes.

Let $Re_0^* = 900$, $Fr = 86$ ($\omega = 0.0774$), and $\beta = 0$ (2-D case). The Orr-Sommerfeld solution provides an eigenvalue

$$\alpha = \alpha_R + i\alpha_I = 0.2229 - i0.00451,$$

and the associated eigenfunctions $\phi_R^x, \phi_T^x, \phi_R^y,$ and $\phi_T^y$ which are dependent only on $y$ (Figure 18).
In LST, the disturbances are assumed to be traveling waves. In the 2-D case, this yields

\begin{align}
    u &= \epsilon e^{-\sigma z} (\phi_R^u \cos(\alpha_R x - \omega_R t) - \phi_T^u \sin(\alpha_R x - \omega_R t)), \\
    v &= \epsilon e^{-\sigma z} (\phi_R^v \cos(\alpha_R x - \omega_R t) - \phi_T^v \sin(\alpha_R x - \omega_R t)).
\end{align}

The inflow boundary velocities can then be obtained by setting \( z = z_0 \) for \( u \) and \( z = z_0 - \frac{\Delta z}{2} \) for \( v \) (\( z_0 \) is the \( z \)-coordinate at inflow). We assume that \( \epsilon \) is small. Figure 18 shows the complex eigenfunctions for both \( u \) and \( v \) components (\( \phi_R^u, \phi_T^u, \phi_R^v, \) and \( \phi_T^v \)) in the physical \((z, y)\) plane, which are normalized by setting \( \max\{\phi_R^u\} = 1 \).

A moderate computational domain is selected. In this case, the plate length (measured from the inflow location \( z = z_0 \)) is set to eleven Tollmien-Schlichting (T-S) wavelengths, while the buffer domain is an additional single wavelength, making the length of the total computational domain twelve T-S wavelengths. Here we choose \( y_{\text{max}} = 75 \) and use a total computational grid with \( 362 \times 50 \) grid points. The grid is highly anisotropic near the solid wall \((\Delta z \gg \Delta y)\).

Since we use a fully-implicit scheme, the time step is restricted mainly by accuracy consideration. For our tests, we take

\[ \Delta t = \frac{2\pi}{320\omega} = 0.2537. \]

The convergence rate of the semi-coarsening multigrid method, which we generally found to be about 0.2 per \( V(2,2) \) cycle (relax twice on each grid level before descending and ascending), is much better than the performance of single-grid relaxation, as shown in Figure 19.
In order to compare the computational results with the linear theory solution, which is accurate for the parallel wall-bounded base flow with small disturbances, we first assume that the base flow is everywhere given by

$$U_0(\xi, \eta) = U_0(0, \eta), \quad V_0(\xi, \eta) = 0, \quad \text{and} \quad \epsilon = 10^{-4},$$

where, $U_0(0, \eta)$ is the Blasius similarity solution in the computational $(\xi, \eta)$ plane at $\xi = 0$ and that the displacement thickness of the boundary layer is a constant, $\delta_{\infty}^*$. Then $Re^* (= Re_0^*)$, $\alpha$, and $\omega$ do not change along the streamwise direction. The streamwise and wall-normal velocity components, $u$ and $v$, of the disturbance after 13 T-S periods ($t = 13T$) are compared with the solutions obtained by the linear theory at a vertical position close to the solid wall ($y^* = 1.3137$ for $u$ and $y^* = 1.2448$ for $v$) in Figure 20. Excellent agreement in both amplitude and phase between the computational results of our fourth-order finite difference scheme and the solution obtained by LST is observed in the physical domain.

Figure 19. Convergence history at a fixed time for multigrid and single-grid relaxation.

Figure 20. Comparison of the numerical and theoretical velocity components near the solid wall ($y^* = 1.3137$ for $u$ and $y^* = 1.2448$ for $v$). $Re^* = 900$, $Fr = 86$, parallel wall-bounded base flow assumption is used grids: 362 x 50 (11 T-S wavelength physical domain + 1 wavelength buffer domain).
To compare our numerical results with those obtained by LST more precisely, we check the profiles of different Fourier modes.

The profiles of the disturbance waves are obtained by using the Fourier transformation. Generally, we can expand any continuous function in the spectral space. Since

\[
\hat{u}(k) = \frac{\omega}{2\pi} \int_{t}^{t+T} \hat{u}(z, y, t)e^{ik\omega t}dt,
\]

where \( \hat{u}(z, y, t) \) is the complex disturbance velocity and \( \hat{u}(k) \) are the Fourier coefficients corresponding to the frequency \( k\omega \), we can then obtain

\[
|\hat{u}(k)| = 2\sqrt{a(k)^2 + b(k)^2}, \quad k = 0, 1, 2, \ldots
\]

with

\[
a(k) = \frac{\omega}{2\pi} \int_{t}^{t+T} \text{Real}{\hat{u}(z, y, t)} \cos(k\omega t)dt,
\]

\[
b(k) = \frac{\omega}{2\pi} \int_{t}^{t+T} \text{Real}{\hat{u}(z, y, t)} \sin(k\omega t)dt.
\]

Only the fundamental wave \( (k = 1) \) is obtained in this case. Figure 21 depicts the streamwise and wall-normal disturbance velocity profiles at \( z^* = 439.2 \) and 608.4 \( (z^* = z/\delta_m) \), and shows the excellent agreement with those obtained by linear stability theory.

![Streamwise disturbance profile of fundamental wave u](image)

![Wall-normal disturbance profile of fundamental wave v](image)

Figure 21. Comparison of the numerical and LST velocity profiles at \( z^* = 439.2 \) and 608.4.

To check the high order accuracy, two different grids \( (362 \times 50 \) and \( 182 \times 26 \) ) are tested. For this kind of unsteady problem, it is quite difficult to show the grid convergence. We define the relative \( L_2 \) error norm for both
and $v$ as

$$||E_u||_2 = \sqrt{\frac{\sum (u - u_*)^2}{\sum u_*^2}},$$

$$||E_v||_2 = \sqrt{\frac{\sum (v - v_*)^2}{\sum v_*^2}},$$

where $u, v$ denote the numerical solution, and $u_*, v_*$ denote the LST solution. The results given in Table I show that the accuracy of our scheme under the above measure is about $O(h^{3.8})$.

| grids   | $||E_u||_2$ | $||E_v||_2$ |
|---------|-------------|-------------|
| $182 \times 26$ | 0.3315 | 0.3243 |
| $362 \times 50$ | 0.0393 | 0.0319 |

Table I. Relative $L_2$ error norm for $u$ and $v$ after 13 T-S periods (calculated in physical domain).

10.2 Secondary instability and transition

Now we return to the real world. The base flow is now not parallel to the solid wall, but the Blasius similarity solution.

The computational domain is restricted to

$$x \in [x_0, x_0 + L_x \lambda_0],$$

$$y \in [0, y_{max}],$$

$$z \in [\pi, 3\pi],$$

where $L_x$ is the number of T-S wavelengths in the computational domain, and $\lambda_0$ is the T-S wavelength at inflow (the T-S wavelength $\lambda$ varies when the base flow is non-parallel).

A Benney-Lin (1960) type disturbance is imposed on the inflow:

$$\tilde{v}(0, y, x, t) = \text{Real}\{\epsilon_{2d}\phi_{2d}^{(k)}(y)e^{i\omega t} + \epsilon_{3d+}\phi_{3d+}^{(k)}e^{i\omega t+i\beta s} + \epsilon_{3d-}\phi_{3d-}^{(k)}e^{i\omega t-i\beta s}\},$$

where $\phi_{2d}(y)$ and $\phi_{3d\pm}(y)$ correspond respectively to 2-D and 3-D eignsolutions of the Orr-Sommerfeld equation and the superscript $(k)$ denotes different velocity components. Following is a typical case we chose:

$$Re_0' = 900, \quad Fr = 86 \quad (\omega = 0.0774),$$

$$\beta = 0.1, \quad y_{max} = 50,$$

$$\alpha_{2d} = 0.2229 - 0.00451i,$$

$$\alpha_{3d} = 0.2169 - 0.00419i,$$

$$\epsilon_{2d} = 0.03, \quad \epsilon_{3d\pm} = 0.01,$$

$$L_x = 10 \quad \text{with 2 T-S wavelengths for buffer domain}$$

$$x_0 = 303.9, \quad z_{end} = 593.6.$$  

The grid we used here is $162 \times 34 \times 34$ (including eight wavelengths and a two wavelength buffer domain). The time step is set to $\frac{1}{280}$ of the 3-D T-S wave period.

It takes around 9 CRAY-YMP CPU hours for the code to run 30 T-S periods. Figures 22 and 23 depict the contours of relative helicity at different times which clearly show the process of K-type fundamental transition, $\lambda$-wave formation, the peak and valley splitting and vortex breakdown. It is found that the breakdown begins at the second peak when the $\lambda$-wave is intensified to certain degree and the shear flow is developed. The vortex breakdown further contaminates the flow field which leads to a transition process. The patterns of helicity at $t = 30T$ is very similar to those $t = 7T$, which suggests that the whole process of transition has been built up after $t = 7T$. It turns out that less than 2 CRAY-YMP hours are needed to simulate the whole process of transition for a $162 \times 34 \times 34$ grid and 7 T-S periods. Figures 24 and 25 give the contour plots of total vorticity magnitude on
the $y = 0.0477$ $(x,z)$-plane and spanwise vorticity on the $z = 31.4$ $(x,y)$-plane at different times which clearly show the process of vortex breakdown and formation of multiple spikes. The appearance of random moving small vortexes after breakdown provides a clue that the flow no longer keeps its laminar status. These contours also show a qualitative agreement with the laboratory experiment conducted by Saric et al. (1984).

The $z$-component of perturbation velocity, $u$, at different streamwise positions, $z = 305, 421, \text{and} 537$, but with same $y$-coordinate ($y = 0.3667$) is shown in Figure 26. Although the disturbance imposed at inflow is a sine function as shown at $z = 305$, the perturbation at other points is largely amplified and distorted. The perturbation velocity no longer keeps its sine function shape, but starts oscillating very fast, showing that high frequency modes have been induced.

We also averaged $u$ and $v$ on $z = 31.4$ $(x,y)$-plane at different streamwise positions, $z = 305, 363, 421, 479, \text{and} 537$ after the transition process was built up. The time-averaged $u$ and $v$ are given in Figures 27, 28, 29, and 30. Figures 28 and 29 depict the differences in $u$ profiles between the Blasius similarity solution and computational results at $z = 421$ and $357$, which qualitatively agree with the experimental results given by Suder, O'Brien, and Reshotko. Figures 28 and 29 also show that the $v$-profile in the transition zone is sharper than those of Blasius solution. The wall stress $\tau = \frac{\partial u}{\partial y}$ is then larger than that of laminar flows.

Figure 30 gives the $v$-profile. The $v$ is always positive in a laminar boundary layer. But, our computational results show that $v$ varies from positive to negative and then becomes positive again. This is a typical sign that the flow is experiencing transition. Figure 31 shows that the spectrum of perturbation $u$ becomes wider as the flow moves downstream. We also tried another case:

$$Re_0^* = 732,$$
$$\omega_{zd} = 0.0909,$$
$$\omega_{zd} = 0.04545,$$
$$\beta = 0.2418, \quad y_{max} = 50,$$
$$\alpha_{zd} = 0.2490 - 0.00351i,$$
$$\alpha_{zd} = 0.1103 - 0.00650i,$$
$$\epsilon_{zd} = 0.015, \quad \epsilon_{zd}^* = 0.005,$$
$$l_s = 10 \text{ with } 2 \text{ T-S wavelengths for buffer domain},$$
$$x_0 = 248.2, \quad x_{end} = 437.5.$$

The grid we used here is still $162 \times 34 \times 34$ (including eight wavelengths and a two wavelength buffer domain). This was set to correspond to a subharmonic transition, but we still got a $k$-type fundamental transition when we chose $\epsilon_{zd} = 0.03$ and $\epsilon_{zd}^* = 0.01$. However, when we changed to $\epsilon_{zd} = 0.015$ and $\epsilon_{zd}^* = 0.005$, a subharmonic transition was very clearly observed (see figure 32).

There is really a lack of reliable experimental data for transitional flow, which can be used to judge the computational results. Also, we need finer grids to get better resolution for post-onset flow or turbulent flow. We have to sacrifice those small eddies now. However, the results apparently provide physically correct simulations for the whole process of flow transition.
Figure 22. Front view of the relative helicity obtained on a $162 \times 34 \times 34$ grid at different times. $Re^* = 900, Fr = 86, \beta = 0.1, \epsilon_{2d} = 0.03, \epsilon_{3d} = 0.01$. Flow direction is from left to right.
Figure 23. Bird view of the relative helicity obtained on a $162 \times 34 \times 34$ grid at different times. $Re^* = 900, Fr = 86, \beta = 0.1, \epsilon_{2d} = 0.03, \epsilon_{3d} = 0.01$. Flow direction is from left to right.
Figure 24. Contour plots of the total vorticity magnitude obtained on a $162 \times 34 \times 34$ grid at different times on the $y_0 = 0.1123$ $(x,z)$-plane. $Re^* = 900, Fr = 86, \beta = 0.1, \epsilon_{2d} = 0.03, \epsilon_{3d} = 0.01$. Contour interval is 0.02, flow direction is from left to right.
Figure 25. Contours plots of spanwise vorticity on the $z_0 = 0$ $(x, y)$-plane at different times. $Re^* = 900$, $Fr = 86$, $\beta = 0.1$, $\epsilon_{\alpha} = 0.03$, $\epsilon_{\beta} = 0.01$.

Contour interval is 0.02, flow direction is from left to right.
Figure 26. Temporal distribution of the perturbation velocity $u$ on $y = 0.367$, $z = 304, 421,$ and 537.

$Re_0^* = 900, Fr = 86, \beta = 0.1, \epsilon_{2d} = 0.03, \epsilon_{3d} = 0.015$. 
Figure 27. Time-averaged $\bar{u}$-profiles at $z = 31, 304, 362, 421, 479,$ and 537. $Re_0 = 900, Fr = 86, \beta = 0.1, \epsilon_{2d} = 0.03, \epsilon_{3d} = 0.01.$

Figure 28. Comparison between $\bar{u}$-profiles and the Blasius profile at $z = 421, x = 31$. $Re_0 = 900, Fr = 86, \beta = 0.1, \epsilon_{2d} = 0.03, \epsilon_{3d} = 0.01.$
Figure 29. Comparison between $\bar{u}$-profile and the Blasius profile at $z = 537$, $x = 31$.
$Re_0 = 900$, $Fr = 86$, $\beta = 0.1$, $\epsilon_{2d} = 0.03$, $\epsilon_{3d} = 0.01$.

Figure 30. Time-averaged $\bar{u}$-profiles at $x = 31$, $x = 304, 362, 421, 479$, and 537.
$Re_0 = 900$, $Fr = 86$, $\beta = 0.1$, $\epsilon_{2d} = 0.03$, $\epsilon_{3d} = 0.01$. 
Figure 31. Streamwise distribution of the $u$-spectrum at $y = 0.715, z = 319.3, 362.8, 406.2, 449.7,$ and $478.6$ $Re_\theta = 900, Fr = 86, \beta = 0.1, \epsilon_2d = 0.03, \epsilon_3d = 0.01i,$ and a $114 \times 34 \times 18$ grid (6 T-S wavelengths physical domain +1 wavelength buffer) is used.
Figure 32. Bird view of the relative helicity of subharmonic transition obtained on a 162 x 34 x 34 grid at different times. $Re^* = 732$, $\beta = 0.2418$, $e_{2d} = 0.015$, $e_{3d} = 0.005$. Flow direction is from left to right.
11 Concluding Remarks

- The fully implicit time-marching and fourth-order finite difference scheme on a stretched and staggered grid is accurate enough to simulate the pre-onset transitional flow with a relatively coarse grid. The computational results agree with linear stability theory, secondary instability theory and some experiments.

- The simulation with relatively coarse grids still can provide qualitatively correct prediction for transitional flow. It shows that the large eddies play more important roles in the process of flow transition.

- The spatial DNS with relatively coarse grids meets trouble at the flow breakdown stage since the grid is not fine enough to resolve the small eddies which play the role to generate dissipations. We then need to introduce some numerical dissipation. The new fine-coarse-fine grid mapping technique can keep the DNS code running to simulate the whole process of transition, including the linear growth, secondary instability, breakdown, and transition.

- To get more accurate DNS simulations, we still need finer grids, especially for post-onset flows.

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References


A new technology was developed in this study which provides a successful numerical simulation of the whole process of flow transition in 3-D boundary layers, including linear growth, secondary instability, breakdown, and transition at relatively low CPU cost. Most other spatial numerical simulations require high CPU cost and blow up at the stage of flow breakdown. A fourth-order finite difference scheme on stretched and staggered grids, a fully implicit time-marching technique, a semi-coarsening multigrid based on the so-called approximate line-box relaxation, and a buffer domain for the outflow boundary conditions were all used for high-order accuracy, good stability, and fast convergence. A new fine-coarse-fine grid mapping technique was developed to keep the code running after the laminar flow breaks down. The computational results are in good agreement with linear stability theory, secondary instability theory, and some experiments. The cost for a typical case with $162 \times 34 \times 34$ grid is around 2 CRAY-YMP CPU hours for 10 T-S periods.