Methods for direct simulation of transition in hypersonic boundary layers II

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1. Motivation and objective

The prediction of transition to turbulence in compressible boundary layers currently receives significant attention due to its importance in the design of high speed transport vehicles. Drag, lift, and heat transfer strongly depend on whether the boundary layer is laminar or turbulent. The study of transition in compressible boundary layers by means of direct numerical simulation (DNS) provides information not available from the commonly used linear and non-linear stability theories. Non-parallel and non-linear effects in the boundary layer can be studied and information useful to modeling of transitional flows can be obtained. The extremely high numerical accuracy and large computing resources necessary for DNS of compressible boundary layers, however, are obstacles to the use of DNS in high Mach number boundary layers.

In our previous report, Van der Vegt and Ferziger (1990), we discussed the development and application of a numerical scheme for the computation of transition in compressible boundary layers. Unfortunately, we encountered serious problems in the application of this method. One problem was related to the generation of initial disturbances, the eigenfunctions of the linear stability problem, needed to start the direct simulations. In a separate paper in this report, Guilyardi et al. (1991), we discuss the problems in solving the linear stability problem with high accuracy for both eigenvalues and eigenfunctions. Previous research has concentrated mainly on the accuracy of the eigenvalues, not on the accuracy in the eigenfunctions. The lack of accurate initial data has seriously hampered progress in the direct simulations. The use of the adaptive method discussed in Van der Vegt and Ferziger (1990) was helpful in generating a grid with enough resolution in the critical layers, but experience with the linear stability problem using several grid adaptation methods showed that the eigenvalue problem is extremely sensitive to the smoothness in the grid. Significant progress has been made by studying the less expensive linear stability problem and is reported in Guilyardi, *et al.* (1991). It is expected that the progress made with adaptive grid generation in the linear stability problem will be helpful in the future development of the DNS code.

In addition to the extensive study of the linear stability problem, a significant effort has been made to increase the accuracy of the numerical algorithm used for direct simulations. In our previous report, Van der Vegt and Ferziger (1990), see also Van der Vegt (1991), we discussed improvements to the upwind numerical scheme

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which reduce the numerical dissipation in the boundary layer region. We want to study flows with both strong shocks and boundary layers, but, unfortunately, most shock capturing schemes are very dissipative in the boundary layer. We presented a fully implicit finite volume method, and significant progress was made in improving the efficiency of a fully implicit method without using the approximate factorization method of Beam and Warming (1978). The finite volume method, however, is only second order accurate, and it was felt that higher order accuracy is necessary in order for success in DNS of transition. The construction of an implicit and time accurate fourth order scheme is the subject of this report.

2. Accomplishments

In order to be useful for direct simulations of transition in boundary layers, the numerical scheme must be higher order accurate and implicit. The severe time step limitation, when using an explicit scheme with small grid spacing close to the wall, would otherwise make the simulations prohibitively expensive. The construction of higher order shock capturing schemes for the Euler and Navier-Stokes equations is a non-trivial task and is currently the subject of intensive research. Significant progress still has to be made. For instance, the numerical scheme used by Rai and Moin (1991) for the direct simulation of bypass transition is higher order accurate, but they are not able to capture shocks because they use a non-conservative formulation. It is very difficult to combine shock capturing without numerical oscillations and uniform higher order accuracy. Many finite volume methods based on the TVD property of the one-dimensional Euler equations are capable of accurately capturing shock and expansion waves with a few grid points. Unfortunately, high order TVD schemes, also called high resolution schemes, break down to first order accuracy at non-sonic local extrema in one dimension and are formally only first order accurate in more than one dimension; see, for instance, Osher and Chakravarthy (1984). In order to bypass this limitation, Harten et al. (1987) developed essentially non-oscillatory (ENO) schemes, which have uniform accuracy away from discontinuities. The application of ENO schemes will be discussed in the next part of this report.

A second important activity has been the implementation of a fully implicit and time accurate integration scheme. This was already discussed in our previous report, Van der Vegt and Ferziger (1990), but changes were made to convert the time integration method to a full Newton scheme. This was necessary because it is not possible to use higher order approximation of the derivatives for the implicit part of the equations when the explicit part is approximated with higher order accuracy. This would reduce the accuracy of the total scheme for time accurate problems, and the higher order accuracy is obtained only when steady state is reached. This approach has also been used by Rai (1987) and Rai and Moin (1991) to reduce the approximate factorization error in their scheme. It turned out that the convergence of the Newton scheme strongly depends on the implementation of the boundary conditions.

2.1 Numerical method

The present algorithm solves the two-dimensional compressible Navier-Stokes equations in conservation form in an arbitrary coordinate system. These can be written:

$$\frac{\partial}{\partial t}\hat{\mathbf{U}} + \frac{\partial}{\partial \xi}(\hat{\mathbf{E}} - \hat{\mathbf{V}}_{vis_\xi}) + \frac{\partial}{\partial \eta}(\hat{\mathbf{G}} - \hat{\mathbf{V}}_{vis_\eta}) = \mathbf{0} \tag{1}$$

with:

$$\hat{\mathbf{U}} = \frac{\mathbf{U}}{J}; \quad \hat{\mathbf{E}} = \frac{\xi_x}{J}\mathbf{E} + \frac{\xi_z}{J}\mathbf{G}; \quad ,\hat{\mathbf{G}} = \frac{\eta_x}{J}\mathbf{E} + \frac{\eta_z}{J}\mathbf{G}$$

$$\hat{\mathbf{V}}_{vis_\xi} = \frac{\xi_x}{J}\mathbf{V} + \frac{\xi_z}{J}\mathbf{I}; \quad \hat{\mathbf{V}}_{vis_\eta} = \frac{\eta_x}{J}\mathbf{V} + \frac{\eta_z}{J}\mathbf{I}$$

and:

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho w \\ e \end{pmatrix}; \quad \mathbf{E} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u w \\ (e+p)u \end{pmatrix}; \quad \mathbf{G} = \begin{pmatrix} \rho w \\ \rho u w \\ \rho w^2 + p \\ (e+p)w \end{pmatrix}$$

$$\mathbf{V} = \frac{1}{Re}\begin{pmatrix} 0 \\ \tau_{xx} \\ \tau_{xz} \\ u\tau_{xx} + w\tau_{xz} - \frac{q_x}{(\gamma-1)M^2 Pr} \end{pmatrix}; \; \mathbf{I} = \frac{1}{Re}\begin{pmatrix} 0 \\ \tau_{xz} \\ \tau_{zz} \\ u\tau_{xz} + w\tau_{zz} - \frac{q_z}{(\gamma-1)M^2 Pr} \end{pmatrix}$$

Here ρ represents the density, u and w the Cartesian velocity components, p the pressure, and e the total energy. The variables x and y represent Cartesian coordinates, whereas ξ and η represent curvilinear coordinates. The coefficients Re, M, and Pr are the Reynolds, Mach, and Prandtl number, respectively. The components of the shear stress τ and heat flux $\mathbf{q}$ in $\mathbf{V}$ and $\mathbf{I}$ are functions of ξ and η. All variables are non-dimensionalized using free-stream variables and a characteristic length.

The Navier-Stokes equations are solved using a finite volume method because we seek a weak solution in order to capture shocks in high Reynolds number flows. The finite volume method is also the most natural way to satisfy the conservation properties of the differential equations. Applying Gauss' theorem and integrating equation (1) over a small volume gives the finite volume formulation of the compressible Navier-Stokes equations:

$$\frac{\partial \overline{\mathbf{U}}_{i,j}}{\partial t} + \overline{\mathbf{E}}_{i+\frac{1}{2},j} - \overline{\mathbf{E}}_{i-\frac{1}{2},j} + \overline{\mathbf{G}}_{i,j+\frac{1}{2}} - \overline{\mathbf{G}}_{i,j-\frac{1}{2}} = \mathbf{0} \tag{2}$$

where a barred quantity with index i,j is an average of the unbarred quantity over the cell with index i,j and indices $i \pm \frac{1}{2}$ and $j \pm \frac{1}{2}$ refer to values at the cell faces.

2.2 Spatial discretization

The computation of the fluxes across the cell faces is the most important part of the numerical scheme. Flux vector or flux difference splitting is used because, in upwind schemes, they automatically generate the proper amount of numerical viscosity in discontinuities, guaranteeing that stable non-oscillatory solutions are obtained when an entropy condition is satisfied, see for instance Osher and Chakravarthy (1984). The upwind method is also very beneficial for the implicit part of the algorithm because it yields a more diagonally dominant matrix suitable for iterative solution. Both Steger-Warming, see Steger and Warming (1981), and Osher flux splitting, see Chakravarthy and Osher (1983), are used. For the implicit part, however, the Steger-Warming splitting is always used because the direct linearization of the Osher flux vector is very expensive and the use of Newton iteration, discussed in the next section, will reduce the error caused by the approximate implicit contribution, see Rai and Chakravarthy (1986). The Steger-Warming splitting has the benefit of being relatively inexpensive, but the Osher splitting is less dissipative. The Osher flux splitting also has the benefit of being Lipschitz continuous, which is important when computing the Jacobian of the flux vector for the implicit contribution. When the Steger-Warming splitting is used, an upwind biased scheme is necessary to reduce the numerical dissipation in the boundary layer, for more details see Van der Vegt (1991).

In order to obtain a higher order scheme, we have to approximate the fluxes at the cell faces by a higher order polynomial. One problem with higher order interpolation in finite volume methods is that we are solving equations for the averaged values in the cells, while needing point values at the cell faces to compute the fluxes. This is referred to as the reconstruction problem by Harten et al. (1987). Using a higher order Newton interpolation scheme based on divided difference tables, they construct a polynomial from the averaged values which is both higher order accurate and conservative. In order to prevent the scheme from using points across a discontinuity, which would give oscillations in the interpolations, they use the divided difference table of the interpolation to determine the stencil which gives the smoothest solution. The ENO scheme, therefore, dynamically adapts its stencil to give uniform higher order accuracy outside discontinuities, and, when combined with a Riemann solver, it captures both shock and expansion waves accurately. The ENO scheme consists of three steps: a reconstruction step, the computation of point values from cell averaged values; the solution of the Riemann problem at the cell faces; and the averaging of the solution to give the cell averaged values.

In one dimension, these methods have been very successful, Harten et al. (1987), especially when used with methods which recognize a shock such as Harten's subcell resolution scheme, Harten (1989). In higher dimensions, however, serious problems occur because the reconstruction becomes very complicated and should in principal be accompanied by a true multi-dimensional Euler solver; the latter are not well developed. Recent progress by Harten and Chakravarthy (1991), however, seems promising.

In order to bypass the problems in formally extending ENO to multi-dimensional

problems, Shu and Osher (1988-1989) proposed the point-ENO method, which applies the ENO method to a series of one-dimensional problems. Their formulation is considerably simpler although less rigorous than that of Harten and Chakravarthy (1991). It has been successfully applied to the study of compressible free shear layers by Shu et al. (1991). As a first step, the higher order scheme is implemented without stencil switching because the boundary complicates the search algorithm and has not been used in the point-ENO method of Shu and Osher. Using an upwind biased fixed interpolation makes it easier to accommodate the boundary and has considerably less numerical dissipation in the boundary layer than a fully upwind scheme. Due to the use of flux splitting, only second order accuracy can be obtained at the boundary. The fact that we do not use the stencil switching temporarily limits the code to flows without shocks.

In order to simplify the development of the numerical scheme, the method of lines, which uncouples the spatial and temporal discretization, is used. The numerical scheme consists of several steps. First, the flux vector is split into a positive and a negative part, depending on the sign of the eigenvalues of the Jacobian matrix of the flux vector:

$$\hat{\mathbf{E}}_{i+\frac{1}{2},j} = \hat{\mathbf{E}}^{+}_{i+\frac{1}{2},j} + \hat{\mathbf{E}}^{-}_{i+\frac{1}{2},j}$$

The positive and negative fluxes at $i+\frac{1}{2},j$ are obtained using a fourth order interpolation formula. The finite volume scheme, however, will always be formally second order accurate, as can be easily checked by Taylor series expansion. The fluxes, therefore, have to be corrected to obtain higher order accuracy in the total scheme. Shu and Osher (1988) derived the following relation:

$$\overline{\mathbf{E}}^{\pm}_{i+\frac{1}{2},j} = \hat{\mathbf{E}}^{\pm}_{i+\frac{1}{2},j} + \sum_{k=1}^{m-1} a_{2k} \Delta\xi^{2k} \left(\frac{\partial^{2k} \hat{\mathbf{E}}^{\pm}}{\partial \xi^{2k}} \right)_{\xi_{i+\frac{1}{2},j}} + O(\Delta\xi^{2m+1})$$

which makes the scheme mth order accurate with coefficients, $a_2 = \frac{-1}{24}$, $a_4 = \frac{7}{5760}, \ldots$. This relation can be obtained using a Taylor series expansion about the point i,j. It has the great benefit of giving a conservative scheme, which converges to a weak solution. This is not necessarily the case when fourth order differences are used. This relation is separately applied to the positive and negative flux vectors by choosing separate polynomial interpolants $p^{\pm}_{i+\frac{1}{2}}$ for $\hat{\mathbf{E}}^{\pm}_{i+\frac{1}{2},j}$, yielding:

$$\overline{\mathbf{E}}^{\pm}_{i+\frac{1}{2},j} = p^{\pm}_{i+\frac{1}{2},j}(\xi_{i+\frac{1}{2},j}) + \sum_{k=1}^{m-1} a_{2k} \Delta\xi^{2k} \left(\frac{\partial^{2k} p^{\pm}_{i+\frac{1}{2},j}}{\partial \xi^{2k}} \right)_{\xi_{i+\frac{1}{2},j}} + O(\Delta\xi^{2m+1}) \quad (3)$$

Similar relations can be derived for the vector $\overline{\mathbf{G}}_{i,j+\frac{1}{2}}$.

2.3 Implicit time integration

Time accuracy is crucial for direct simulations. Unfortunately, most implicit schemes do not have this property. In an effort to improve time accuracy, Rai (1987) proposed to use a Newton iteration to improve the time accuracy of approximate factorization schemes. This was applied by Rai and Moin (1991) in their simulations of bypass transition in a boundary layer at Mach 0.1. By recomputing the Jacobian matrix, they reduce the approximate factorization error and increase time accuracy. We do not use approximate factorization or ADI to solve the implicit matrix but the zebra line Gauss-Seidel method. This method converges very rapidly (in two to three iterations) and gives a solution of the full system of linear equations. We do not need Newton iteration to remove the inaccuracy introduced by approximate factorization, but because the Jacobian matrix is only approximated to first order in the implicit part, we do not achieve time accuracy and lose the higher order spatial accuracy of the scheme. Linearization of the equations with a higher order implicit spatial discretization is not feasible because it requires a prohibitively large amount of storage. The Newton time integration method, therefore, is needed to maintain time accuracy. It is obtained by including the flux vectors at time level $n+1$ in Equation (2) and applying the Newton-Raphson iteration process. To save space we only discuss the one-dimensional form:

$$\left(\alpha I + J\triangle t\left(\frac{\partial \overline{\mathbf{E}}^p}{\partial \mathbf{U}_{i+\frac{1}{2},j}} - \frac{\partial \overline{\mathbf{E}}^p}{\partial \mathbf{U}_{i-\frac{1}{2},j}}\right)\right)\left(\mathbf{U}^{p+1} - \mathbf{U}^p\right) = -T\left(\mathbf{U}^p, \mathbf{U}^n, \mathbf{U}^{n-1}, \ldots\right) - J\triangle t\left(\overline{\mathbf{E}}^p_{i+\frac{1}{2},j} - \overline{\mathbf{E}}^p_{i-\frac{1}{2},j}\right) \tag{4}$$

Where T and α depend on the time integration method used. For instance, a first order implicit time integration uses $\alpha = 1$ and

$$T\left(\mathbf{U}^p, \mathbf{U}^n\right) = \left(\mathbf{U}^p - \mathbf{U}^n\right)$$

whereas as second order time integration uses $\alpha = \frac{3}{2}$ and

$$T\left(\mathbf{U}^p, \mathbf{U}^n, \mathbf{U}^{n-1}\right) = \left(\frac{3}{2}\mathbf{U}^p - 2\mathbf{U}^n + \frac{1}{2}\mathbf{U}^{n-1}\right)$$

The flux vectors on the right-hand side of Equation (4) are approximated with the higher order scheme, whereas the terms on the left-hand side are only approximated to first order. By iterating the solution of Equation (4) and updating both the implicit and explicit parts each time, we can reduce the error $\mathbf{U}^{p+1} - \mathbf{U}^p$ to zero and thereby obtain a higher order implicit and time accurate scheme. In practice only a few iterations are needed.

Higher order time integration methods can be obtained by using higher order difference approximations for $\frac{\partial \mathbf{U}}{\partial t}$, but their application becomes more complicated due to the number of time levels, which have to be stored. In two dimensions,

we experimented with accuracy up to fourth order, but the results were not satisfactory. Spurious modes, which arise in multi-level schemes, created instabilities. The spurious modes arise because the characteristic polynomial of the time integration scheme has multiple zeros. A scheme which does not have this problem is the implicit Runge-Kutta method, see for instance Gear (1971). It also has the benefit of having $2m$ order accuracy with only m time levels, see Butcher (1964). A fourth order implicit Runge-Kutta method, which uses only two time levels, is currently being investigated as an alternative. It requires the solution of a large set of non-linear equations and fits in naturally into the Newton scheme. However, it doubles the number of non-linear equations compared with higher order multi-step methods.

Another aspect of the Newton scheme is the fact that the boundary conditions have to be implemented in a Newton form. This can be done straightforwardly using the approach of Chakravarthy (1983). For the inviscid part of the flow field, this procedure can be summarized as follows: Multiply the equations by the left eigenvector of the Jacobian of the inviscid flux vector component normal to the boundary. It is then possible to transform the equations from conservative to characteristic variables. Retaining only the equations which relate to waves which leave the domain and replacing the other equations with boundary conditions yields the equations which have to be solved at the boundary with the Newton method:

$$\begin{pmatrix} (C_{\hat{\mathbf{E}}}S)_k \\ \left(\frac{\partial \mathbf{B}}{\partial \mathbf{U}}\right)_l \end{pmatrix} \frac{\partial U}{\partial t} + \begin{pmatrix} (C_{\hat{\mathbf{E}}}S)_k \\ 0 \end{pmatrix} \left(\frac{\partial \hat{\mathbf{E}}}{\partial \xi} + \frac{\partial \hat{\mathbf{G}}}{\partial \eta} \right) + \begin{pmatrix} 0 \\ \mathbf{B}_l \end{pmatrix} = \mathbf{0}$$

with: $(C_{\hat{\mathbf{E}}}S)_k$ the $k = 1, \ldots, q$ rows of the left eigenvector of the Jacobian of the flux vector $\hat{\mathbf{E}}$ related to outgoing waves; and $\left(\frac{\partial \mathbf{B}}{\partial \mathbf{U}}\right)_l$ and $\mathbf{B}_l$, the $l = q+1, \ldots m$ rows of $\frac{\partial \mathbf{B}}{\partial \mathbf{U}}$ and the vector $\mathbf{B}$ related to the boundary conditions. A similar approach can be followed for the viscous boundary conditions, but an ad hoc decision must be made on which equations to replace by boundary conditions because there is no theory equivalent to the characteristic approach for the inviscid equations available.

3. Discussion

The numerical scheme discussed in this report has been programmed and is currently being tested. The Newton scheme converges, but the residue reduces only linearly instead of quadratically. This is because the implicit part only uses a first order accurate approximation to the spatial derivatives, which are approximated with higher order accuracy on the right hand side. Convergence problems, however, sometimes occur due to the corner contributions; removing them requires additional attention. Another problem which still is under investigation is point to point oscillations which occur in low Mach number inviscid flow. These oscillations disappear as soon as the viscous contribution is incorporated, even with a very low viscosity, but they also should not occur at all. The convergence of the Newton scheme is a very good test of the code because it is very sensitive to any error in the code.

4. Future plans

The present version of the code will have to be tested further, and work has to be completed on the elimination of the weak instability. When the code is operational, both spatial and temporal simulations of boundary layer transition will be performed. The experience gained using the adaptive grid method in the linear stability code will also be applied. It is expected that the increased accuracy of the DNS and linear stability code will be sufficient to perform DNS simulations of transition in compressible boundary layers at reasonable cost.

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REFERENCES

BEAM, R. M. & WARMING, R. F. 1978 An Implicit Factored Scheme for the Compressible Navier-Stokes Equations. *AIAA Journal.* **16**, 393-402.

BUTCHER, J. C. 1964 Implicit Runge-Kutta Processes. *Mathematics of Computation.* **18**, 50-64.

CHAKRAVARTHY, S. R. 1983 Euler Equations - Implicit Schemes and Boundary Conditions. *AIAA Journal.* **21**, 699-706.

CHAKRAVARTHY, S. R. & OSHER, S. 1983 Numerical Experiments with the Osher Upwind Scheme for the Euler Equations. *AIAA Journal.* **21**, 1241-1248.

GUILYARDI, E., VAN DER VEGT, J. J. W. & FERZIGER, J. H. 1991 Linear Stability Analysis of Hypersonic Boundary Layers. *Annual Research Briefs,* Center for Turbulence Research, Stanford University.

HARTEN, A., ENGQUIST, B., OSHER, S. & CHAKRAVARTHY S. R. 1987 Uniform High Order Accurate Essentially Non-Oscillatory Schemes III. *Journal of Computational Physics.* **71**, 231-303.

HARTEN, A., 1989 ENO Schemes with Subcell Resolution. *Journal of Computational Physics.* **83**, 148-184.

HARTEN, A. & CHAKRAVARTHY, S. R. 1991 Multi-Dimensional ENO Schemes for General Geometries. ICASE Report 91-76, NASA Langley.

OSHER, S. & CHAKRAVARTHY, S. R. 1984 High Resolution Schemes and the Entropy Condition. *SIAM Journal on Numerical Analysis.* **21**, 955-984.

RAI, M. M. & CHAKRAVARTHY, S. R. 1986 An Implicit Form for the Osher Upwind Scheme. *AIAA Journal.* **24**, 735-743.

RAI, M. M. 1987 Navier-Stokes Simulations of Blade-Vortex Interaction using High-Order Accurate Upwind Schemes. AIAA paper 87-0543.

RAI, M. M. & MOIN, P. 1991 Direct Numerical Simulation of Transition and Turbulence in a Spatially Evolving Boundary Layer. AIAA paper 91-1607-CP.

SHU, C. W. AND OSHER, S. 1988 Efficient Implementation of Essentially Non-Oscillatory Shock-Capturing Schemes. *J. of Comp. Physics.* **77**, 439-471.

SHU, C. W. AND OSHER, O. 1989 Efficient Implementation of Essentially Non-Oscillatory Shock Capturing Schemes II. *Journal of Computational Physics.* **83,** 32-78.

SHU, C. W., ERLEBACHER, G., ZANG, T. A., WHITAKER, D. & OSHER, S. 1991 High-Order ENO Schemes Applied to Two- and Three-Dimensional Compressible Flow. ICASE Report, 91-38, NASA Langley.

STEGER, J. L. & WARMING, R. F. 1981 Flux-Vector Splitting of the Inviscid Gasdynamic Equations with Application to Finite-Difference Methods. *Journal of Computational Physics.* **40,** 263-293.

VAN DER VEGT, J. J. W. 1991 Assessment of Flux Vector Splitting for Viscous Compressible Flows. AIAA Paper 91-0243.

VAN DER VEGT, J. J. W. & FERZIGER, J. H. 1990 Methods for Direct Simulation of Transition in Hypersonic Boundary Layers. *Annual Research Briefs,* Center for Turbulence Research, Stanford University.