

Implicit Computation of Three-Dimensional Compressible Navier–Stokes Equations Using k – ϵ Closure

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A computational method for the numerical integration of the Favre–Reynolds-averaged three-dimensional compressible Navier–Stokes equations using the Launder–Sharma near-wall k – ϵ turbulence closure is developed. The mean flow and turbulence transport equations are discretized using a finite volume method based on MUSCL Van Leer flux-vector splitting with Van Albada limiters. The mean flow and turbulence equations are integrated in time using a fully coupled approximately factored implicit backward Euler method. The resulting scheme is robust and was found stable for local-time steps with Courant–Friedrichs–Lewy number equal to 50. Higher time steps are possible but not optimal for convergence. Results are presented for the three Déclery transonic channel test-cases. Although these test-cases are nominally two dimensional, three-dimensional computations presented quantify the important three-dimensional effects induced by the sidewall boundary layers. Finally computational results are compared with the experiment for a geometrically three-dimensional transonic nozzle.

Introduction

NEAR-WALL two-equation turbulence models^{1–8} are increasingly used in computational fluid dynamics (CFD), and it is hoped that some of their modeling drawbacks will be corrected by the use of more advanced models^{9–11} including near-wall Reynolds-stress models^{12–16} and compressibility effects.^{17–21} The interest in using transport-equation models of turbulence in CFD is the result not only of their higher accuracy in complex configurations but also of the simpler computer logic involved with comparison to zero-equation models. The authors believe that near-wall turbulence models are more interesting for CFD purposes than the wall-functions approach, although opinion on this is divided.^{22–24}

The major problem of codes using transport-equation models of turbulence in the transonic regime (including shock-wave/boundary-layer interaction) is their robustness and, as a consequence, their computational efficiency. A satisfactory method should run from a simple automatic initialization of the flowfield and have the same convergence characteristics, in terms of Courant–Friedrichs–Lewy (CFL) number²⁵ (time marching schemes) or relaxation parameters (pressure-based schemes and Newton-iteration procedures), as their zero-equation model counterparts, as well as exhibit robustness characteristics analogous to zero-equation model methods. The last point is a major item and, if achieved, transport-equation models will presumably definitely replace zero-equation models, at least for complex three-dimensional configurations where the implementation of models using such concepts as distance from the wall and profile extremum is delicate.

This work is not concerned so much with turbulence modeling as with the efficient numerical implementation of low-Reynolds near-wall two-equation models. An overview of methods using two-equation models in the transonic regime, including a summary of their computational characteristics, is interesting (Table 1).^{26–77} This overview is certainly not exhaustive and is mostly based on AIAA Journal articles, but the authors believe it is quite representative of the evolution of the state of the art over the past 10 years. The nondimensional distance from the wall of the first grid point nearest to it, $n_w^+ = n \nu_w^{-1} \sqrt{(\tau_w / \rho_w)}$ (where n is the distance from the wall, τ_w the resultant wall shear stress, ρ_w the density

at the wall, and ν_w the kinematic viscosity at the wall), is a very important grid-resolution parameter. Most workers (Table 1) acknowledge that, in the transonic régime ($M < 2?$), values of $n_w^+ < 1$ are necessary to obtain accurate grid-independent results.

Practically all methods can be augmented by a multigrid procedure to achieve higher computational efficiency.^{43,49–52} Independent of this, the admissible CFL number is an approximate gauge of the computational rapidity of time-marching methods. This is not true for relaxation methods where time does not appear explicitly, nor for the hybrid MacCormack scheme. Neither of these methods can be readily extended to unsteady flows. When time-marching methods are considered, it appears that the average CFL number used is ~ 5 (Table 1). Increasing the optimal CFL number has a nonlinear accelerating effect on convergence and is, therefore, highly desirable. Unsteady flow computations consistently use much higher CFL numbers that are stable in the highly stretched grids used without local time-stepping (for consistency), and will not be considered here.^{78–82} There are three published methods that appear more advanced than the others. Coakley³⁰ and Lin et al.⁵⁸ achieved CFL = 8 using upwind discretizations with implicit approximate factorization. Lin et al.⁵⁸ achieved CFL = 70 using a nonfactored implicit method, but the cost/iteration is about three times greater than factored methods. A more important problem of nonfactored methods is that computer-memory-requirements are 1 order of magnitude greater (compared with factored methods in three-dimensions).

There are, unfortunately, few authors who analyze the problems associated with the numerical implementation of two-equation models. The use of limiters was introduced by Coakley and Viegas,²⁷ who used minimum bounds and a maximum–minimum turbulence length-scale concept to ensure positivity and boundedness of turbulence variables (k , ϵ , or ω). Other authors^{43,45,46,51,52,57} used analogous limiters, often also limiting the production of turbulence kinetic energy P_k with respect to its dissipation ϵ to avoid non-physical overshoots in the neighborhood of the shock wave. One of the few systematic attempts to analyze the stability of k – ϵ solvers was reported by Kunz and Lakshminarayana.⁴⁶ There seems to be some doubt concerning whether source terms are stiff or not, what their importance on stability is, and whether their implicit treatment is necessary, different authors reporting contradictory conclusions. There is not necessarily a unique answer to these questions, since the interaction between the numerical scheme, the limiters, and the model should be considered as an integrated system and not separately. A review of the literature and practical experience tend to point out that (although the authors are unable to prove this mathematically) upwind schemes are more robust for treating the convection of turbulence variables; limiters are most important at the boundary-layer edge, where production and dissipation decrease

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Table 1 Time-marching methods for transonic Navier–Stokes with two-equation closure and local-time-stepping

References	Date	Two/three dimensional	Model (Ref.)	Space	Time	CFL	n_w^+
27–29	1977	Two dimensional	$k-\varepsilon(3)$	MacCormack ⁵⁹	Hybrid ⁵⁹	—	5
30	1985	Two dimensional	$q-\omega(7)$	Coakley ³⁰	SR ³ implicit ³⁰	5–8	0.8
31	1986	Two dimensional	$k-\varepsilon(3)$	MacCormack ⁵⁹	Hybrid ⁵⁹	—	?
32–34	1986	Three dimensional	$k-\varepsilon(3)$	MacCormack ⁵⁹	Explicit ⁵⁹	<1	WF ^b
35–38	1986	Three dimensional	$k-\varepsilon(3)$	MacCormack ⁵⁹	Hybrid ⁵⁹	—	0.3–0.7
39	1986	Two dimensional	$k-\varepsilon(6)$	Beam–Warming ⁶⁰	AF ^c implicit	?	1
40	1988	Two dimensional	$k-\varepsilon(26)$	Hopscotch ⁶²	Explicit ⁶¹	<1	WF
41	1989	Three dimensional	$q-\omega(7)$	Coakley ³⁰	SR implicit ³⁰	3–5	1
42	1990	Three dimensional	$k-\varepsilon(26)$	Jameson ⁶³	SR implicit ⁴²	4–6	WF
43	1990	Two dimensional	$k-\varepsilon(5)$	Ni ⁶⁵	SR implicit ⁶⁶	3	0.2
44	1991	Two dimensional	$k-\varepsilon(6)$	Quick ⁶⁴	PB ^d 44	—	1–5
45	1992	Two dimensional	$k-\varepsilon(6)$	Jameson ⁶³	Explicit RK ^c 63	$2\sqrt{2}$	1
46	1992	Three dimensional	$k-\varepsilon(6)$	Jameson ⁶³	Explicit RK ⁶³	$2\sqrt{2}$	1
47	1992	Two dimensional	$k-\varepsilon(5)$	MacCormack ⁵⁹	Explicit ⁵⁹	0.4–0.8	1
48	1992	Two dimensional	$q-\omega(7)$	Jameson ⁶³	SR implicit ^{30,60}	5?	1
49	1993	Two dimensional	$k-\varepsilon$	Ni ⁶⁵	Explicit ⁶⁵	<1	1
50	1993	Two dimensional	$k-\varepsilon(50)$	Quick ⁶⁷	Explicit PB ⁵⁰	<1?	1
51, 52	1993	Three dimensional	$k-\varepsilon$	Jameson ⁶³	Explicit RK ⁶³	$2\sqrt{2}$	WF
53	1994	Three dimensional	$k-\varepsilon(5)$	Beam–Warming ⁶⁰	AF implicit ⁶⁰	5	1
54	1994	Two dimensional	$k-\varepsilon(8)$	Liu and Jameson ⁶⁸	Explicit RK ⁶³	5?	0.5–2
55	1995	Three dimensional	$k-\varepsilon(3)$	Lax–Wendroff ⁶⁹	Explicit ⁶³	<1	3
56	1995	Two dimensional	$k-\varepsilon(8)$	Roe ^{70,71}	Explicit RK63	3?	0.5–2
57	1995	Three dimensional	$k-\varepsilon(26)$	unstructured ⁵⁷ Roe	SR implicit ^{63,72}	2	WF
58	1995	Two dimensional	$k-\varepsilon(6)$	Yee–Harten ⁷³	AF implicit ⁵⁸	8?	0.55
58	1995	Two dimensional	$k-\varepsilon(6)$	Yee–Harten ⁷³	NF ^f implicit ⁵⁸	70?	0.55
Present	1996	Three dimensional	$k-\varepsilon(5)$	Van Leer ^{74,75}	AF implicit ^{76,77}	50	0.5

^aSR = spectral radius. ^bWF = wall functions. ^cAF = approximately factored. ^dPB = pressure based. ^eRK = Runge–Kutta. ^fNF = nonfactored.

rapidly, and diffusion balances convection (an interesting analysis of the associated instability is given by Stüttgen and Peters⁸³), and not, as is often stated by wall-function users, in the near-wall region; and the importance of the implicit treatment of source terms depends strongly on the scheme used.

The purpose of this work is to develop a fully coupled implicit upwind scheme for the three-dimensional compressible Navier–Stokes equations, combining computational efficiency and computational robustness. The method is based on Van Leer MUSCL discretization^{74,75} of the convective terms, with factored implicit time integration.^{76,77} The Jacobian operator of the implicit step is approximated by a first-order upwind scheme for the convective fluxes, and a spectral-radius matrix for the viscous fluxes. The source-terms are simply factored, without using any special procedure, such as suggested by Shih and Chyu,⁸⁴ or positivity fixes.³¹ Optimal convergence is obtained for CFL = 50. The method is applied to the computation of several transonic channel flows.

Flow Model and Computational Method

Flow Model

The flow is modeled by the compressible Favre–Reynolds-averaged^{85,86} three-dimensional Navier–Stokes equations, with a compressible flow extension to the Launder–Sharma⁵ near-wall $k-\varepsilon$ closure:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j}{\partial x_j} = 0 \quad (1)$$

$$\frac{\partial \bar{\rho} \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} [\bar{\rho} \bar{u}_i \bar{u}_j + \bar{p} \delta_{ij}] - \frac{\partial (\bar{\tau}_{ij} - \bar{\rho} \bar{u}_i' \bar{u}_j')}{\partial x_j} = 0 \quad (2)$$

$$\begin{aligned} \frac{\partial (\bar{\rho} \bar{h}_t - \bar{p})}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j \bar{h}_t}{\partial x_j} - \frac{\partial}{\partial x_j} [\bar{u}_i (\bar{\tau}_{ij} - \bar{\rho} \bar{u}_i' \bar{u}_j')] \\ - (\bar{q}_j + \bar{\rho} \bar{e}'' \bar{u}_j'') + P_k - \bar{\rho} \varepsilon^* - 2\mu \frac{\partial \sqrt{k}}{\partial x_j} \frac{\partial \sqrt{k}}{\partial x_j} = 0 \end{aligned} \quad (3)$$

$$\begin{aligned} \frac{\partial \bar{\rho} k}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j k}{\partial x_j} - \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_T}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] \\ - P_k + \bar{\rho} \varepsilon^* + 2\mu \frac{\partial \sqrt{k}}{\partial x_j} \frac{\partial \sqrt{k}}{\partial x_j} = 0 \end{aligned} \quad (4)$$

$$\begin{aligned} \frac{\partial \bar{\rho} \varepsilon^*}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j \varepsilon^*}{\partial x_j} - \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_T}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon^*}{\partial x_j} \right] - C_{\varepsilon 1} P_k \frac{\varepsilon^*}{k} \\ + C_{\varepsilon 2} f_{\varepsilon 2} \bar{\rho} \frac{\varepsilon^{*2}}{k} - 2 \frac{\mu \mu_T}{\bar{\rho}} \left(\frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} \right) \left(\frac{\partial^2 \bar{u}_i}{\partial x_\ell \partial x_\ell} \right) = 0 \end{aligned} \quad (5)$$

$$\begin{aligned} \bar{p} = \bar{\rho} R_g \bar{T} = \bar{\rho} \frac{\gamma - 1}{\gamma} \bar{h} = \bar{\rho} (\gamma - 1) \bar{e} \\ - \bar{\rho} \bar{u}_i' \bar{u}_j'' = \mu_T \left[\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right] - \frac{2}{3} \mu_T \frac{\partial \bar{u}_j}{\partial x_j} \delta_{ij} - \frac{2}{3} \bar{\rho} k \delta_{ij} \end{aligned} \quad (6)$$

$$\begin{aligned} \bar{\tau}_{ij} \cong \mu (\bar{T}) \left[\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right] - \frac{2}{3} \mu \frac{\partial \bar{u}_j}{\partial x_j} \delta_{ij} \\ P_k = -\frac{1}{2} \bar{\rho} \bar{u}_i' \bar{u}_j'' \left[\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right]; \quad \bar{q}_i \cong -\kappa (\bar{T}) \frac{\partial \bar{T}}{\partial x_i} \end{aligned} \quad (7)$$

$$\bar{\rho} \bar{e}'' \bar{u}_j'' = -\kappa_T \frac{\partial \bar{T}}{\partial x_j}$$

where t is the time, x_i the Cartesian space coordinates, \bar{u}_i the velocity components, $\bar{\rho}$ the density, \bar{p} the pressure, \bar{T} the temperature, \bar{h} the enthalpy, $\gamma = 1.4$ the isentropic exponent, $R_g = 287.04 \text{ m}^2 \text{ s}^{-2} \text{ K}^{-1}$ the gas constant for air, $\bar{h}_t = \bar{h} + \frac{1}{2} \bar{u}_i \bar{u}_i$ the total enthalpy of the mean flow (which is different from $\bar{h}_t = \bar{h}_t + k$), k the turbulence kinetic energy, ε^* the isotropic part of the turbulence kinetic-energy dissipation rate ($\varepsilon^* \doteq \varepsilon - 2\nu [\text{grad} \sqrt{k}]^2$, where ε is the dissipation rate, and ν the kinematic viscosity), $\bar{\tau}_{ij}$ the viscous stress tensor, μ the molecular dynamic viscosity, μ_T the eddy viscosity, κ the molecular heat conductivity, and κ_T the eddy heat conductivity; $\bar{\cdot}$ denotes Favre averaging, and $\bar{\cdot}$ denotes nonweighted averaging. The near-wall terms, accounting for the anisotropic part of the dissipation rate, in the k equation ($2\mu [\text{grad} \sqrt{k}]^2$) and in the ε equation ($2\nu \mu_T [\nabla^2 \bar{V}]^2$), are written in Cartesian tensor form, independently of the wall distance or orientation.^{2,43,45} The model constants and the molecular diffusion coefficients are

$$\begin{aligned} C_{\varepsilon 1} = 1.44; \quad C_{\varepsilon 2} = 1.92; \quad \sigma_k = 1; \quad \sigma_\varepsilon = 1.3 \\ f_{\varepsilon 2}(Re_T) = 1 - 0.3e^{-Re_T^2}; \quad Re_T \doteq k^2/\nu \varepsilon^* \end{aligned} \quad (8)$$

$$\frac{d\mathbf{w}_{i,j,k}}{dt} \approx -\frac{1}{\mathcal{V}_{i,j,k}} \left[\begin{array}{l} +^{\xi} \mathcal{S}_{i+\frac{1}{2},j,k} \left[\mathbf{F}^+ \left(\xi \mathbf{w}_{i+\frac{1}{2},j,k}^-, \xi \mathbf{n}_{i+\frac{1}{2},j,k} \right) + \mathbf{F}^- \left(\xi \mathbf{w}_{i+\frac{1}{2},j,k}^+, \xi \mathbf{n}_{i+\frac{1}{2},j,k} \right) + {}^{\vee} \mathbf{F}_{i+\frac{1}{2},j,k} \cdot \xi \mathbf{n}_{i+\frac{1}{2},j,k} \right] \\ -^{\xi} \mathcal{S}_{i-\frac{1}{2},j,k} \left[\mathbf{F}^+ \left(\xi \mathbf{w}_{i-\frac{1}{2},j,k}^-, \xi \mathbf{n}_{i-\frac{1}{2},j,k} \right) + \mathbf{F}^- \left(\xi \mathbf{w}_{i-\frac{1}{2},j,k}^+, \xi \mathbf{n}_{i-\frac{1}{2},j,k} \right) + {}^{\vee} \mathbf{F}_{i-\frac{1}{2},j,k} \cdot \xi \mathbf{n}_{i-\frac{1}{2},j,k} \right] \\ +^{\eta} \mathcal{S}_{i,j+\frac{1}{2},k} \left[\mathbf{F}^+ \left(\eta \mathbf{w}_{i,j+\frac{1}{2},k}^-, \eta \mathbf{n}_{i,j+\frac{1}{2},k} \right) + \mathbf{F}^- \left(\eta \mathbf{w}_{i,j+\frac{1}{2},k}^+, \eta \mathbf{n}_{i,j+\frac{1}{2},k} \right) + {}^{\vee} \mathbf{F}_{i,j+\frac{1}{2},k} \cdot \eta \mathbf{n}_{i,j+\frac{1}{2},k} \right] \\ -^{\eta} \mathcal{S}_{i,j-\frac{1}{2},k} \left[\mathbf{F}^+ \left(\eta \mathbf{w}_{i,j-\frac{1}{2},k}^-, \eta \mathbf{n}_{i,j-\frac{1}{2},k} \right) + \mathbf{F}^- \left(\eta \mathbf{w}_{i,j-\frac{1}{2},k}^+, \eta \mathbf{n}_{i,j-\frac{1}{2},k} \right) + {}^{\vee} \mathbf{F}_{i,j-\frac{1}{2},k} \cdot \eta \mathbf{n}_{i,j-\frac{1}{2},k} \right] \\ +^{\zeta} \mathcal{S}_{i,j,k+\frac{1}{2}} \left[\mathbf{F}^+ \left(\zeta \mathbf{w}_{i,j,k+\frac{1}{2}}^-, \zeta \mathbf{n}_{i,j,k+\frac{1}{2}} \right) + \mathbf{F}^- \left(\zeta \mathbf{w}_{i,j,k+\frac{1}{2}}^+, \zeta \mathbf{n}_{i,j,k+\frac{1}{2}} \right) + {}^{\vee} \mathbf{F}_{i,j,k+\frac{1}{2}} \cdot \zeta \mathbf{n}_{i,j,k+\frac{1}{2}} \right] \\ -^{\zeta} \mathcal{S}_{i,j,k-\frac{1}{2}} \left[\mathbf{F}^+ \left(\zeta \mathbf{w}_{i,j,k-\frac{1}{2}}^-, \zeta \mathbf{n}_{i,j,k-\frac{1}{2}} \right) + \mathbf{F}^- \left(\zeta \mathbf{w}_{i,j,k-\frac{1}{2}}^+, \zeta \mathbf{n}_{i,j,k-\frac{1}{2}} \right) + {}^{\vee} \mathbf{F}_{i,j,k-\frac{1}{2}} \cdot \zeta \mathbf{n}_{i,j,k-\frac{1}{2}} \right] \end{array} \right] - \mathcal{S}_{i,j,k} \quad (14)$$

$$\mu_T = C_\mu f_\mu(Re_T) \mu Re_T; \quad C_\mu = 0.09$$

$$f_\mu(Re_T) = \exp \left[\frac{-3.4}{(1 + 0.02 Re_T)^2} \right] \quad (9)$$

$$\kappa_T = \mu_T c_p / Pr_T; \quad Pr_T = 0.9$$

$$\mu(\tilde{T}) = \mu_{273} \left[\frac{\tilde{T}}{273.15} \right]^{\frac{3}{2}} \frac{110.4 + 273.15}{110.4 + \tilde{T}} \quad (10)$$

$$\kappa(\tilde{T}) = \kappa_{273} [\mu(\tilde{T}) / \mu_{273}] [1 + 0.00023(\tilde{T} - 273.15)]$$

where $\mu_{273} = 17.11 \times 10^{-6}$ Pa s, and $\kappa_{273} = 0.0242$ W m⁻¹ K⁻¹.

Note that a source term is present in the mean-flow energy equation [Eq. (3)]. This term is necessary because the averaging operator $\bar{\rho} \tilde{h}_t = \bar{\rho} h + (1/2) \bar{\rho} u_i u_i = \bar{\rho} \tilde{h}_t + \bar{\rho} k$ introduces the turbulence kinetic energy $k = (1/2) \bar{u}_i'' \bar{u}_i''$. Several authors include this term by introducing a modified pressure $p^* = \bar{p} + \frac{2}{3} \bar{\rho} k$ (Refs. 31 and 55), whereas others neglect it since it becomes important only in high-supersonic flows.^{43,45} This new formulation introduces the correct fully coupled mean-flow energy equation, while avoiding the modified-pressure formulation.

Space-Discretization

These equations [Eqs. (1–5)] are discretized on a structured grid using a finite volume technique, with vertex storage. Defining the vector of unknowns \mathbf{w} (not to be confused with the velocity component w)

$$\mathbf{w} = [\bar{\rho}, \bar{\rho} \tilde{u}, \bar{\rho} \tilde{v}, \bar{\rho} \tilde{w}, \bar{\rho} \tilde{h}_t, -\bar{p}, \bar{\rho} k, \bar{\rho} \varepsilon^*]^T \in \mathbb{R}^7 \quad (11)$$

the Navier–Stokes [Eqs. (1–3)] and turbulence-transport equations [Eqs. (4) and (5)] can be written

$$\frac{\partial \mathbf{w}}{\partial t} + \text{div}[\mathbf{C}\mathbf{F}(\mathbf{w}) + {}^{\vee}\mathbf{F}(\mathbf{w}) + \mathbf{S}(\mathbf{w})] = 0 \quad (12)$$

where the convective fluxes $\mathbf{C}\mathbf{F} \in \mathbb{R}^7 \otimes \mathbb{R}^3$, the viscous fluxes ${}^{\vee}\mathbf{F} \in \mathbb{R}^7 \otimes \mathbb{R}^3$, and the source terms $\mathbf{S}(\mathbf{w}) \in \mathbb{R}^7$ are easily identified from Eqs. (1–5). The divergence of convective fluxes is discretized using the flux-vector-splitting method of Van Leer⁷⁵ with third-order MUSCL interpolation⁷⁴ and Van Albada limiters.⁸⁷ The divergence of viscous fluxes is computed using the centered scheme described by Arnore.⁸⁸ The present implementation follows closely the work of Anderson et al.^{76,77} Defining a staggered grid

$$\begin{aligned} \mathbf{x}_{i \pm \frac{1}{2}, j \pm \frac{1}{2}, k \pm \frac{1}{2}} &= \frac{1}{8} [\mathbf{x}_{i,j,k} + \mathbf{x}_{i \pm 1, j, k} + \mathbf{x}_{i \pm 1, j \pm 1, k} + \mathbf{x}_{i, j \pm 1, k} \\ &+ \mathbf{x}_{i, j, k \pm 1} + \mathbf{x}_{i \pm 1, j, k \pm 1} + \mathbf{x}_{i \pm 1, j \pm 1, k \pm 1} + \mathbf{x}_{i, j \pm 1, k \pm 1}] \end{aligned} \quad (13)$$

and noting (ξ, η, ζ) the grid directions (i, j, k) , $(\xi \mathcal{S}_{i \pm (1/2), j, k}, \eta \mathcal{S}_{i, j \pm (1/2), k}, \zeta \mathcal{S}_{i, j, k \pm (1/2)})$ the cell-face areas of the staggered-grid cell around the point (i, j, k) , and $(\xi \mathbf{n}_{i \pm (1/2), j, k}, \eta \mathbf{n}_{i, j \pm (1/2), k}, \zeta \mathbf{n}_{i, j, k \pm (1/2)})$ the corresponding normals, the semidiscrete scheme can be written

where $\mathcal{V}_{i,j,k}$ is the control-volume computed as the sum of 6 pyramids.⁸⁹ The viscous fluxes at cell-faces are given by

$$\begin{aligned} {}^{\vee} \mathbf{F}_{i \pm \frac{1}{2}, j, k} &= \frac{1}{2} [{}^{\vee} \mathbf{F}_{i, j, k} + {}^{\vee} \mathbf{F}_{i \pm 1, j, k}] \\ {}^{\vee} \mathbf{F}_{i, j \pm \frac{1}{2}, k} &= \frac{1}{2} [{}^{\vee} \mathbf{F}_{i, j, k} + {}^{\vee} \mathbf{F}_{i, j \pm 1, k}] \\ {}^{\vee} \mathbf{F}_{i, j, k \pm \frac{1}{2}} &= \frac{1}{2} [{}^{\vee} \mathbf{F}_{i, j, k} + {}^{\vee} \mathbf{F}_{i, j, k \pm 1}] \end{aligned} \quad (15)$$

and the Van Leer fluxes are given by

$$\begin{aligned} \mathbf{F}^{\pm} &= \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \\ &\quad \pm M_n(\mathbf{w}, \mathbf{n}) < -1 \\ &\quad \underbrace{\begin{bmatrix} 1 \\ n_x(a/\gamma)(-M_n \pm 2) + \tilde{u} \\ n_y(a/\gamma)(-M_n \pm 2) + \tilde{v} \\ n_z(a/\gamma)(-M_n \pm 2) + \tilde{w} \\ \frac{-(\gamma - 1)M_n^2 \pm 2(\gamma - 1)M_n + 2}{\gamma^2 - 1} a^2 + \frac{\tilde{V}^2}{2} \\ k \\ \varepsilon^* \end{bmatrix}}_{|M_n(\mathbf{w}, \mathbf{n})| \leq 1} \\ &\quad \underbrace{\begin{bmatrix} \bar{\rho} \tilde{V}_n \\ \bar{\rho} \tilde{V}_n \tilde{u} + \bar{p} n_x \\ \bar{\rho} \tilde{V}_n \tilde{v} + \bar{p} n_y \\ \bar{\rho} \tilde{V}_n \tilde{w} + \bar{p} n_z \\ \bar{\rho} \tilde{V}_n \tilde{h}_t \\ \bar{\rho} \tilde{V}_n k \\ \bar{\rho} \tilde{V}_n \varepsilon^* \end{bmatrix}}_{\pm M_n(\mathbf{w}, \mathbf{n}) > 1} \end{aligned} \quad (16)$$

where $M_n(\mathbf{w}, \mathbf{n}) = \tilde{V}(\mathbf{w}) \cdot \mathbf{n} / a(\mathbf{w}) = \tilde{V}_n / a$ and $a(\mathbf{w}) = \sqrt{[\gamma R_g \tilde{T}(\mathbf{w})]}$. The MUSCL variables are given by

$$\begin{aligned} \mathbf{w}_{i - \frac{1}{2}, j, k}^{\pm} &= \mathbf{w}^{\pm} \left(\mathbf{w}_{i - \frac{3}{2} \pm \frac{1}{2}, j, k}, \mathbf{w}_{i - \frac{1}{2} \pm \frac{1}{2}, j, k}, \mathbf{w}_{i + \frac{1}{2} \pm \frac{1}{2}, j, k} \right) \\ \mathbf{w}_{i, j - \frac{1}{2}, k}^{\pm} &= \mathbf{w}^{\pm} \left(\mathbf{w}_{i, j - \frac{3}{2} \pm \frac{1}{2}, k}, \mathbf{w}_{i, j - \frac{1}{2} \pm \frac{1}{2}, k}, \mathbf{w}_{i, j + \frac{1}{2} \pm \frac{1}{2}, k} \right) \\ \mathbf{w}_{i, j, k - \frac{1}{2}}^{\pm} &= \mathbf{w}^{\pm} \left(\mathbf{w}_{i, j, k - \frac{3}{2} \pm \frac{1}{2}}, \mathbf{w}_{i, j, k - \frac{1}{2} \pm \frac{1}{2}}, \mathbf{w}_{i, j, k + \frac{1}{2} \pm \frac{1}{2}} \right) \end{aligned} \quad (17)$$

where the MUSCL interpolation \mathbf{w}^\pm and the Van Albada limiters s are

$$\begin{aligned} \mathbf{w}^\pm(\mathbf{w}_{-1}, \mathbf{w}_0, \mathbf{w}_{+1}) &= \mathbf{w}_0 \mp \{(\pm/4)[1 \mp (\pm/3)](\mathbf{w}_{+1} - \mathbf{w}_0) \\ &\quad + (\pm/4)[1 \pm (\pm/3)](\mathbf{w}_0 - \mathbf{w}_{-1})\} \\ s(\mathbf{w}_{-1}, \mathbf{w}_0, \mathbf{w}_{+1}) &= \\ &= \frac{2\text{dif}(\mathbf{w}_{+1}, \mathbf{w}_0) \cdot \text{dif}(\mathbf{w}_0, \mathbf{w}_{-1}) + 10^{-23}}{\text{dif}(\mathbf{w}_{+1}, \mathbf{w}_0) \cdot \text{dif}(\mathbf{w}_{+1}, \mathbf{w}_0) + \text{dif}(\mathbf{w}_0, \mathbf{w}_{-1}) \cdot \text{dif}(\mathbf{w}_0, \mathbf{w}_{-1}) + 10^{-23}} \end{aligned} \quad (18)$$

where the 10^{-23} term is introduced to avoid division by 0 and

$$\text{dif}(\mathbf{w}_A, \mathbf{w}_B) = \left[\frac{\bar{\rho}_A - \bar{\rho}_B}{\rho_{AB}}, \frac{\bar{\rho}_A \bar{u}_A - \bar{\rho}_B \bar{u}_B}{\rho_{AB} a_{AB}}, \frac{\bar{\rho}_A \bar{v}_A - \bar{\rho}_B \bar{v}_B}{\rho_{AB} a_{AB}}, \frac{\bar{\rho}_A \bar{w}_A - \bar{\rho}_B \bar{w}_B}{\rho_{AB} a_{AB}}, \frac{(\bar{\rho}_A \bar{h}_{tA} - \bar{\rho}_A) - (\bar{\rho}_B \bar{h}_{tB} - \bar{\rho}_B)}{\rho_{AB} a_{AB}^2}, 0, 0 \right]^T \quad (19)$$

where $\rho_{AB} = \frac{1}{2}(\bar{\rho}_A + \bar{\rho}_B)$ and $\frac{1}{2}(a_A + a_B)$. The nondimensional differences are necessary because the present code is written directly in SI units, contrary to the usual nondimensional practice. Appropriate extrapolations are used at the boundaries of the computational domain.⁹⁰ Viscous stresses are computed using a centered second-order finite difference scheme.⁸⁸

Time Integration

Denoting by $\mathcal{L}_{i,j,k}$ the discretized form of the space operator (divergence and source terms), the semi discrete equation at grid-point (i, j, k) gives

$$\frac{d\mathbf{w}_{i,j,k}}{dt} + \mathcal{L}_{i,j,k} \mathbf{w} \cong 0 \quad \forall i, j, k \iff \frac{d\mathbf{w}}{dt} + \mathcal{L}(\mathbf{w}) \cong 0 \quad (20)$$

where $\mathbf{w} = [\mathbf{w}_{1,1,1}, \mathbf{w}_{1,1,2}, \dots, \mathbf{w}_{N_i, N_j, N_k}]^T \in \mathbb{R}^{7 \times N_i \times N_j \times N_k}$ and $\mathcal{L} = [\mathcal{L}_{1,1,1}, \mathcal{L}_{1,1,2}, \dots, \mathcal{L}_{N_i, N_j, N_k}]^T \in \mathbb{R}^{7 \times N_i \times N_j \times N_k}$ are the global vectors of the unknowns and space operators. The time discretization of the semidiscrete scheme uses a first-order implicit scheme, and can be written between instants n and $n+1$

$$\left(\mathcal{I} + \Delta t \frac{\partial \mathcal{L}}{\partial \mathbf{w}} \right)^{(n+1)} \mathbf{w} - {}^n \mathbf{w} \cong -\Delta t \mathcal{L}({}^n \mathbf{w}) \quad (21)$$

where $\mathcal{I} \in \mathbb{R}^{(7 \times N_i \times N_j \times N_k) \times (7 \times N_i \times N_j \times N_k)}$ is the identity matrix and the Jacobian matrix $\partial \mathcal{L} / \partial \mathbf{w}$ is evaluated at time n . Any approximation of the system matrix will retain formal first-order time-accuracy, which is sufficient for steady computations. The resulting linear system is solved after approximate factorization of the Jacobian matrix of convective and viscous fluxes and source terms. The bandwidth of the spacewise systems is reduced using a spatially first-order accurate approximation for the implicit term. Viscous terms are treated using a spectral radius approximation.

$$\begin{aligned} \Delta t_{i,j,k} {}^\xi \mathbf{A}_{i+1,j,k} {}^\xi \Delta \mathbf{w}_{i+1,j,k} + (1 + \Delta t_{i,j,k} {}^\xi \mathbf{A}_{i,j,k}) {}^\xi \Delta \mathbf{w}_{i,j,k} \\ + \Delta t_{i,j,k} {}^\xi \mathbf{A}_{i-1,j,k} {}^\xi \Delta \mathbf{w}_{i-1,j,k} = -\Delta t_{i,j,k} {}^n \mathcal{L}_{i,j,k} \\ \Delta t_{i,j,k} {}^\eta \mathbf{A}_{i,j+1,k} {}^\eta \Delta \mathbf{w}_{i,j+1,k} + (1 + \Delta t_{i,j,k} {}^\eta \mathbf{A}_{i,j,k}) {}^\eta \Delta \mathbf{w}_{i,j,k} \\ + \Delta t_{i,j,k} {}^\eta \mathbf{A}_{i,j-1,k} {}^\eta \Delta \mathbf{w}_{i,j-1,k} = {}^\xi \Delta \mathbf{w}_{i,j,k} \\ \Delta t_{i,j,k} {}^\zeta \mathbf{A}_{i,j,k+1} {}^\zeta \Delta \mathbf{w}_{i,j,k+1} + (1 + \Delta t_{i,j,k} {}^\zeta \mathbf{A}_{i,j,k}) {}^\zeta \Delta \mathbf{w}_{i,j,k} \\ + \Delta t_{i,j,k} {}^\zeta \mathbf{A}_{i,j,k-1} {}^\zeta \Delta \mathbf{w}_{i,j,k-1} = {}^\eta \Delta \mathbf{w}_{i,j,k} \\ \left(1 + \Delta t_{i,j,k} \frac{\partial S}{\partial \mathbf{w}}({}^n \mathbf{w}_{i,j,k}) \right) \Delta \mathbf{w}_{i,j,k} = {}^\zeta \Delta \mathbf{w}_{i,j,k} \end{aligned} \quad (22)$$

The three successive spacewise linear systems are solved using banded lower-upper (LU) factorization.⁹¹ The corresponding bandwidth is $(1 + 2 \times 13)$. The implicit phase for the source-terms involves only the local inversion of a 2×2 matrix. The 7×7 real matrices ${}^{\xi, \eta, \zeta} \mathbf{A}_{i \pm 1, j \pm 1, k \pm 1}$, ${}^{\xi, \eta, \zeta} \mathbf{A}_{i, j, k}$, $\partial S / \partial \mathbf{w}$, are given in Vallet.⁹²

Local Time Step

The local time step is based on a combined convective (Courant) and viscous (von Neumann) criterion⁴⁶:

$$\begin{aligned} \Delta t_{i,j,k} &\leq \\ \text{CFL} \min \left\{ \frac{\ell_g}{\tilde{V} + a\sqrt{1 + (5/3)(\gamma - 1)(k/a^2)}}, \frac{\ell_g^2}{2\nu_{\text{eq}}} \right\} \forall i, j, k \\ \nu_{\text{eq}} &= \max \left\{ \frac{4}{3}(\nu + \nu_T), [(\gamma - 1)/\rho R_g](\kappa + \kappa_T) \right\} \end{aligned} \quad (23)$$

where ℓ_g is the grid cell size, \tilde{V} the flow velocity, a the sound velocity, and ν_{eq} the equivalent diffusivity, computed by MacCormack.⁵⁹ Note that the turbulence Mach number¹⁸ $M_T = \sqrt{(2\kappa a^{-2})}$ appears in the convective stability time step, as has been demonstrated by many authors.^{27,31,46} The particular form used here was given recently by Raulot⁹³ and is based on a one-dimensional stability analysis. For steady computations, a CFL = 50 is used with local time stepping.

Boundary Conditions

To achieve the high time steps used and the associated rapid convergence rate, it is indispensable to apply boundary conditions both implicitly and explicitly. The following boundary conditions were implemented.

Inflow reservoir condition:

$$\begin{aligned} \frac{\partial \tilde{s}}{\partial t} = 0; \quad \frac{\partial \tilde{h}_t}{\partial t} = 0; \quad \frac{\partial [\tilde{V} - (\tilde{V} \cdot \mathbf{n})\mathbf{n}]}{\partial t} = 0 \\ \frac{\partial k}{\partial t} = 0; \quad \frac{\partial \varepsilon^*}{\partial t} = 0 \end{aligned} \quad (24)$$

Adiabatic wall condition:

$$\tilde{V} = 0; \quad \frac{\partial \tilde{p}}{\partial n} = 0; \quad \frac{\partial \tilde{T}}{\partial n} = 0; \quad k = 0; \quad \varepsilon^* = 0 \quad (25)$$

Outflow pressure condition:

$$\begin{aligned} \frac{\partial \tilde{p}}{\partial t} = 0; \quad \frac{\partial \tilde{p}}{\partial n} = 0; \quad \frac{\partial \tilde{V}}{\partial n} = 0 \\ \frac{\partial k}{\partial n} = 0; \quad \frac{\partial \varepsilon^*}{\partial n} = 0 \end{aligned} \quad (26)$$

Plane-of-symmetry condition:

$$\frac{\partial \mathbf{w}}{\partial n} = 0; \quad \tilde{\mathbf{V}} \cdot \mathbf{n} = 0 \quad (27)$$

where $\tilde{s} = s(\tilde{p}, \tilde{T})$ is the entropy and \mathbf{n} the unit normal to the boundary. The inflow boundary condition is implemented using the theory of finite waves⁹⁴ and is treated implicitly following the corrections method of Chakravarthy,⁹⁵ to account for the outgoing pressure wave.

Initialization

The authors believe that for practical purposes a Navier–Stokes solver must be able to start from a simple initialization of the flow-field. For stability it is best to fit analytic flat-plate profiles at solid boundaries. These profiles are fitted to a simple inviscid flowfield obtained by linearly interpolating pressure between inflow and outflow, and assuming isentropic adiabatic evolution. The mean flow and turbulence profiles are obtained analytically in a manner similar to that of Gerolymos.⁴³ In the case of solid corners, the two-dimensional profiles are extended to three dimensional using a simple blending rule, based on the distance from the walls. The details for the initialization procedure are given in Vallet.⁹²

k - ε Positivity and Boundedness

To ensure the stability of the method, it is necessary to introduce limiters for k and ε , which may otherwise diverge towards nonphysical values. The following very simple and particularly efficient limiters were used:

$$\text{if } \{k < 0 \vee \varepsilon^* < 0 \vee \ell_T \div (k^{\frac{3}{2}}/\varepsilon^*) > \ell_{T_{\max}}\} : \{k \leftarrow 0 \wedge \varepsilon^* \leftarrow 0\} \quad (28)$$

where $\ell_{T_{\max}}$ is a maximum admissible length scale (a characteristic order-of-magnitude length of the configuration). Divisions by 0 are avoided throughout the code by adding 10^{-23} to the denominator [e.g., when $k = 0$ and $\varepsilon^* = 0$, $k^2/\varepsilon^* \cong k^2/(\varepsilon^* + 10^{-23}) = 0$ and $\varepsilon^{*2}/k \cong \varepsilon^{*2}/(k + 10^{-23}) = 0$]. Also, following Turner and Jennions⁵¹ and Jennions and Turner,⁵² the production of turbulence kinetic energy was limited to twice the dissipation:

$$P_k \leftarrow \min\{P_k, 2\rho\varepsilon^*\} \quad (29)$$

These simple positivity and boundedness fixes stabilize the computations in all of the cases studied in this paper and also in more complex configurations such as wings and turbomachinery cascades.⁹⁶ They are less stringent and more effective than the limiters used previously by Gerolymos,⁴³ the main advantage coming from fixing k and ε^* to 0 and not appropriating small values as is usually done.^{27,43,45,46}

Results

Configurations Studied

The numerical method described in this paper was applied to several transonic channel configurations (Table 2), for which experimental measurements were available.^{55,97,98} The first three configurations are nominally two dimensional, although as will be shown in the following, they are contaminated by three-dimensional effects, because of the shock-wave/boundary-layer interaction at the channel-corners. The last configuration is fully three dimensional (geometrically). Because of paper length limitations, only a few of the results detailed in Vallet⁹² are presented.

Two-Dimensional Results for D  lery Nozzles

Initial computations were run in pseudo-two-dimensional mode using the three-dimensional code. For these computations five equidistant mesh planes were used in the lateral direction (z wise) with symmetry conditions on the sidewalls. The computational grid is generated algebraically. It consists of planes perpendicular to the x axis, equidistant between the inflow and outflow stations. In the y

direction the mesh is stretched geometrically. The same y_w^+ is used on both the upper and lower walls, with the same geometric-progression ratio r_y , so that (with the constraint N_j odd) the upper and lower wall progressions match at half-distance. The two-dimensional results⁹² are typical for these configurations and agree with results obtained with different numerical methods.^{43,49,50}

Influence of n_w^+ and CFL Number on Results

To demonstrate that results are independent of time step, computations for D  lery B nozzle, using the fine 177×193 grid with $y_w^+ = 0.45$ (Table 3), were run for CFL numbers 40, 50, 60, and 80. Comparison of the isentropic wall Mach-number distributions shows⁹² that there is practically no dependence on time step, whereas consideration of the number of iterations to convergence (Table 4) indicates that CFL ~ 50 is nearly optimal.

The importance of grid refinement on results has been discussed recently by Roache,⁹⁹ who introduced the important concept of grid-convergence index. This concept is unfortunately not applicable as such to the grids used in this study because the grids are dependent on two parameters, the number of points (N_i , N_j , N_k) and the size of the first cell nearest the wall n_w^+ . Practical experience of virtually all users of near-wall turbulence closures (e.g., Table 1) suggests that n_w^+ is the most important parameter concerning grid quality. In other words the grids necessary for near-wall turbulence closures depend both on linear refinement (for the away from the wall regions) and on the nonlinear one associated with the viscous sublayer resolution. This nonlinear refinement is characterized by the stretching used (exponential, geometric) and n_w^+ . To illustrate this point pseudo-two-dimensional computations were run, for the D  lery A nozzle using four different grids with the same x -wise resolution ($N_i = 129$), which differ in the y direction (Table 3). The first two grids have both $N_j = 129$, but one ($N_j = 129$, $y_w^+ = 0.41$) is more stretched than the other ($N_j = 129$, $y_w^+ = 1.09$), which is evidently finer away from the wall (Fig. 1). Then two other grids ($N_j = 115$, $y_w^+ = 1.00$) and ($N_j = 111$, $y_w^+ = 1.50$) were used that have the same mesh size at the nozzle axis as the ($N_j = 129$, $y_w^+ = 0.41$) grid but are less stretched. Such grids are often tempting to industrial users, as they permit less expensive computations, not only because they have less points (an effect that is more pronounced in three dimensions) but also because the coarser near-wall mesh means higher time steps and associated faster convergence (less iterations). Consideration of results (Fig. 1) shows clearly that the single most important parameter is n_w^+ . Grids ($N_j = 129$, $y_w^+ = 1.09$) and ($N_j = 115$, $y_w^+ = 1.00$) give practically identical results, although the second is coarser at the axis. In general, lower n_w^+ corresponds to lower computed viscous losses

Table 2 Configurations studied

Case	Description	$L_x \times L_y \times L_z$, mm	M_{shock}	Chord (χ , mm)	Re_χ	Computation
D��lery A ⁹⁷	Two symmetric bumps	$500 \times 100 \times 120.0$	1.30	200	2.0×10^6	Two dimensional
D��lery B ⁹⁷	Two symmetric bumps	$550 \times 100 \times 120.0$	1.45	269	2.5×10^6	Two and three dimensional
D��lery C ⁹⁷	Bump on lower wall	$500 \times 100 \times 120.0$	1.36	286	2.8×10^6	Two dimensional
D��lery three dimensional ^{55,98}	Three-dimensional bump on lower wall	$800 \times 100 \times 121.3$	1.83	245–370	$2.2\text{--}3.3 \times 10^6$	Three dimensional

Table 3 Computational grids summary

Case	$N_i(N_x)$	$N_j(N_y)$	$N_k(N_z)$	y_w^+	z_w^+	r_y	r_z	Computation
D��lery A	129	129	5	0.41	—	1.1500	—	Pseudo-two dimensional
	129	129	5	1.09	—	1.1300	—	Pseudo-two dimensional
	129	115	5	1.00	—	1.1550	—	Pseudo-two dimensional
	129	111	5	1.50	—	1.1525	—	Pseudo-two dimensional
	177	193	5	0.41	—	1.0920	—	Pseudo-two dimensional
D��lery B	129	129	5	0.38	—	1.1500	—	Pseudo-two dimensional
	177	193	5	0.45	—	1.0900	—	Pseudo-two dimensional
	161	65	65	0.48	0.46	1.1450	1.1500	Three dimensional
	161	65	97	0.48	0.46	1.1450	1.0920	Three dimensional
	129	129	5	0.40	—	1.1500	—	Pseudo-two dimensional
D��lery C	177	193	5	0.50	—	1.0900	—	Pseudo-two dimensional
	121	49	49	1.50	1.50	1.5100	1.4440	Three dimensional
D��lery three dimensional	201	91	101	0.75	0.75	1.2155	1.1935	Three dimensional

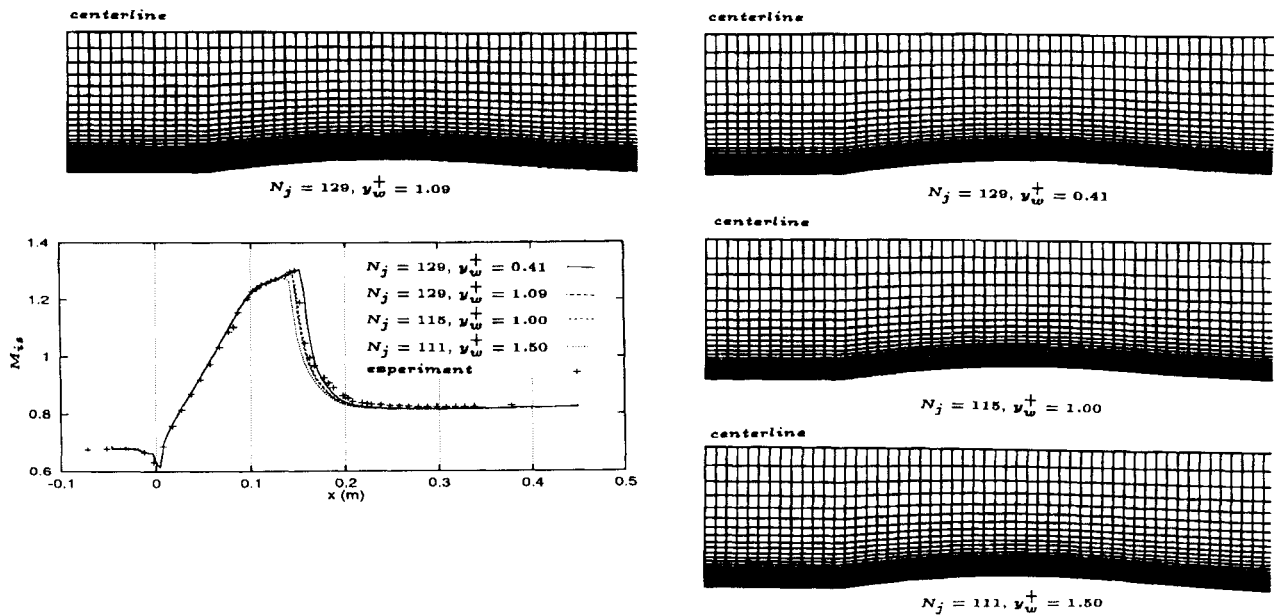


Fig. 1 Influence of n_w^+ on results for Déclery A nozzle.

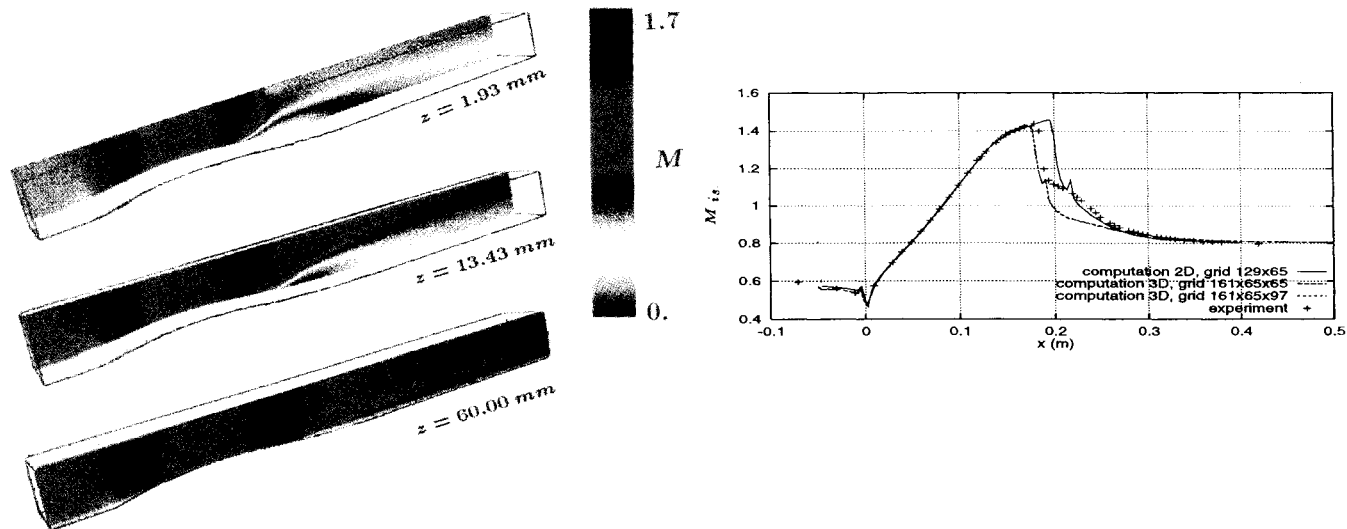


Fig. 2 Comparison of two- and three-dimensional computations with experiment for Déclery B nozzle.

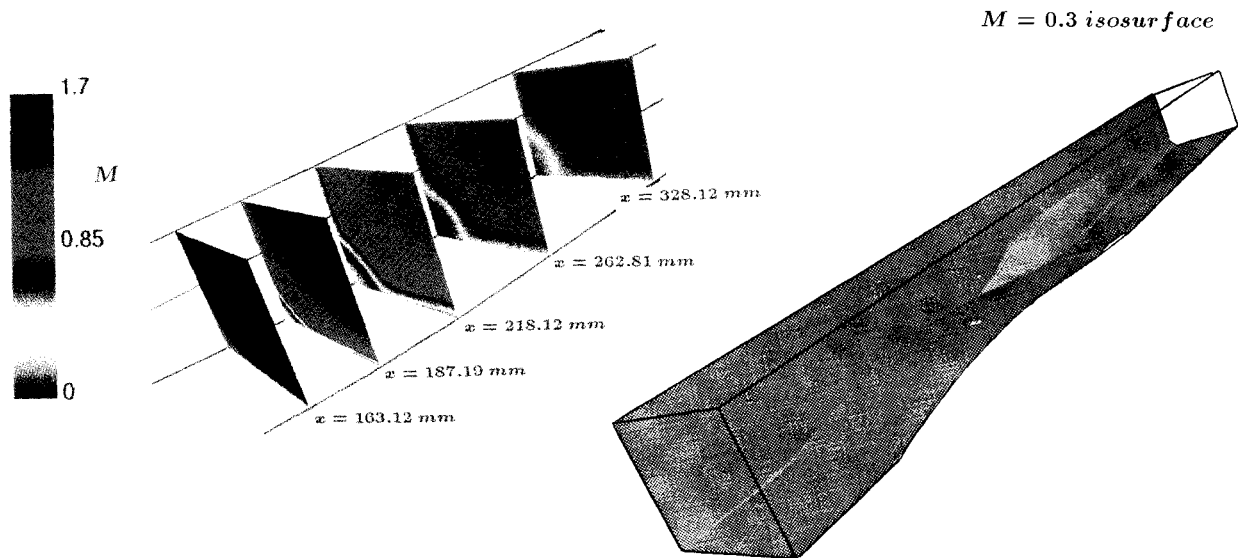


Fig. 3 Three-dimensional separation at the sidewall corner for Déclery B nozzle.

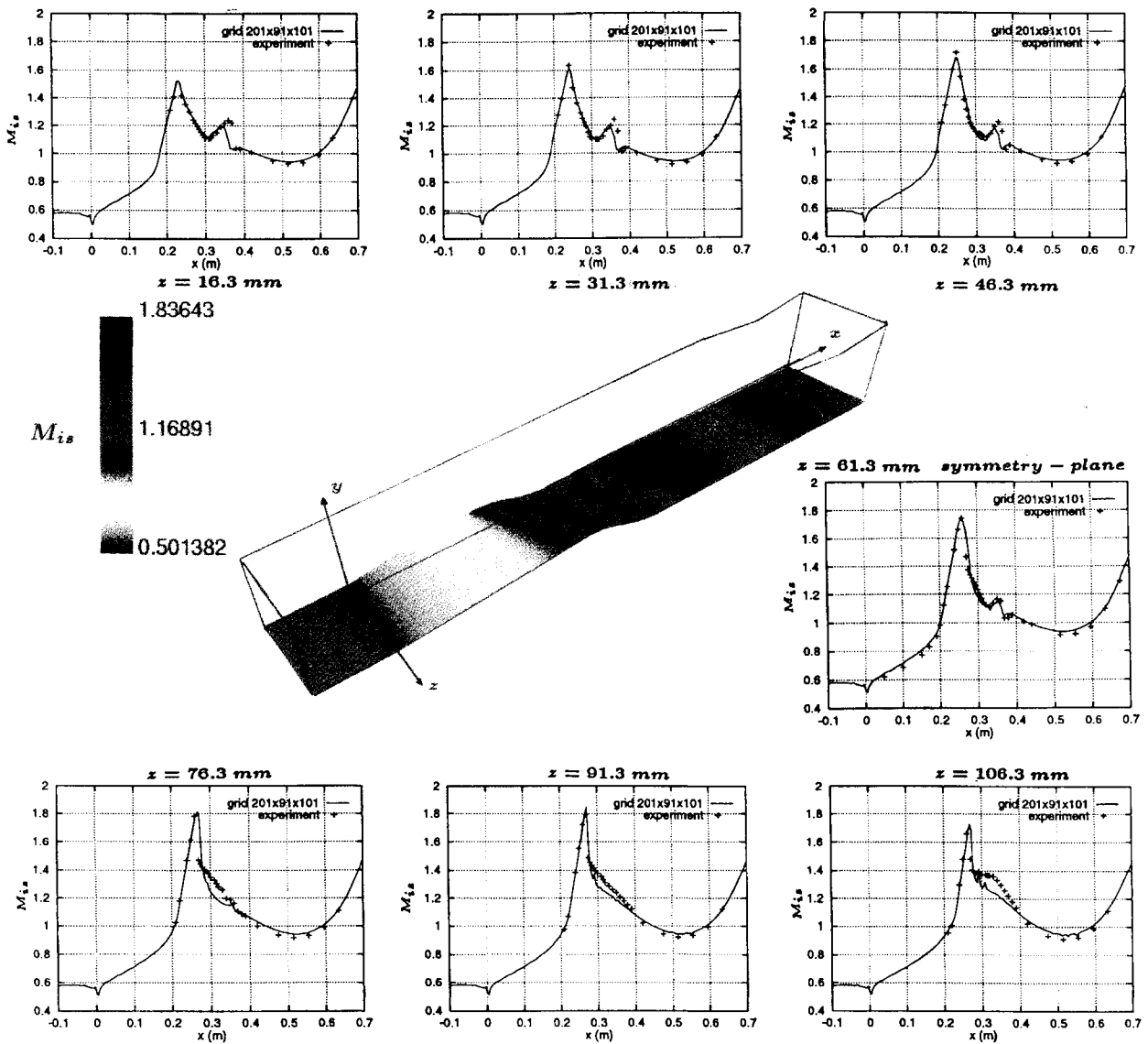
Fig. 4 M_{isw} distributions for Déleré three-dimensional nozzle.

Table 4 Influence of CFL number on convergence

CFL	Iterations to convergence
40	1600
50	1400
60	2000
80	2000

and as a consequence a more downstream position of the shock wave.

Three-Dimensional Effects for Déleré B Nozzle

To assess the importance of three-dimensional effects for Déleré B nozzle three-dimensional computations were run. Only $\frac{1}{4}$ of the nozzle was discretized, and symmetry conditions were imposed at the y - and z -wise symmetry planes. The grid was stretched both y wise and z wise as described in the two-dimensional computations section. Computations were run with two grids (Table 3) for which $y_w^+ \cong z_w^+ \cong 0.5$. For both grids the mesh at the y -symmetry plane is identical with the one used for the pseudo-two-dimensional computations (notice that now only one-half of the nozzle height is discretized so that 65 points correspond to $\frac{1}{2}$ of 129, and that the outflow boundary was placed farther downstream). Both grids yield identical results (Fig. 2), showing that no further z -wise refinement is necessary.

There is a substantial difference in isentropic wall Mach-number distribution between the three-dimensional and the pseudo-



Fig. 5 Iso-Machs for Déleré three-dimensional nozzle.

two-dimensional computations (Fig. 2), suggesting that three-dimensional effects are substantial. This is clearly seen in the isoplots of Mach number at three different positions away from the sidewall (Fig. 2) that suggest the presence of important boundary-layer separation at the corner between the lower wall and the sidewall, because of the three-dimensional shock-wave/boundary-layer interaction. This interaction is better understood considering

Table 5 Computing time requirements for three-dimensional computations

Case	Grid ($N_i \times N_j \times N_k$)	M points ^a	M words	y_w^+	z_w^+	Iterations	CPU, h ^b
Délery B	$161 \times 65 \times 65$	0.65	53	0.48	0.46	900	14
	$161 \times 65 \times 97$	0.97	82	0.48	0.46	1000	21
Délery three dimensional	$121 \times 49 \times 49$	0.28	25	1.50	1.50	300	3
	$201 \times 91 \times 101$	1.76	141	0.75	0.75	900	31

^a One M points = 1024^2 . ^b Cray C-98.

the iso-Machs at various x -wise planes, in the neighborhood of the interaction (Fig. 3) illustrating the detachment and reattachment of the boundary layer. The surface on which $\bar{M} = 0.3$ (Fig. 3) shows clearly the displacement effect on the sidewall. This three-dimensional effect induces a shock wave that is much farther upstream than the one computed on the assumption that the flow is two dimensional. The comparison of the three-dimensional computation with experiment is fair but far from satisfactory. Although the shock wave is now placed at almost the right position (Fig. 2), the subsequent boundary-layer detachment is grossly underestimated, because of the inadequacy of the k - ϵ model.

Délery Three-Dimensional Nozzle

This configuration consists of a swept three-dimensional bump on the lower wall. The upper wall is slightly sloped downward, and the two sidewalls are parallel planes. As in all preceding cases the experimental setup includes an adjustable second throat, which is used to generate and adjust the shock wave.^{97,98} Contrary to the usual computational practice of imposing a constant back pressure (which was also used in the preceding sections) it was preferred to include the second throat in the computations. The flow is accelerated to a supersonic exit, and the shock-wave position is adjusted by the second throat area. Initial tests using a very coarse $\sim 0.28M$ points grid (Table 3) were used to determine the throat height.

Results using a $\sim 1.76M$ points grid (Table 3) with $y_w^+ = z_w^+ = 0.75$ show quite satisfactory agreement with the measured isentropic wall Mach-number distributions on the lower wall (Fig. 4). The agreement is remarkable at the symmetry plane ($z = 61.3$ mm) where the λ shock wave is accurately predicted. The agreement is fair but less satisfactory near the sidewalls. Toward the far wall (shorter bump) there appears, in both the experiment and the computations, the λ shock-wave structure, but although the position of the first shock wave is well predicted, the computations underestimate the strength of the second shock wave. Toward the near wall (longer bump) the shock wave is stronger and the computations underestimate the detachment of the boundary layer after the interaction and fail to predict the pressure-plateau at the near-wall corner.

The flow structure is shown in the iso-Machs plots (Fig. 5). There is a large recirculation zone at the lower wall near the corner because of the strong shock wave ($M_{isw} \sim 1.8$), whereas the flow remains attached at the far corner. The shock wave on the upper wall is quite strong ($M_{isw} \sim 1.65$), and there is a noticeable boundary-layer separation that spans the entire channel width.

Computing Time Requirements

The code runs on a Cray C-98 computer. Its vectorization is adequate but not outstanding (~ 250 Mflops), and computing-time requirements (Table 5) can still be substantially reduced. The computing time necessary for the pseudo-two-dimensional computations is not presented because it cannot be compared with two-dimensional methods (five transverse planes are used). Note that a deliberate choice was made to minimize memory requirements, even at a small sacrifice of computational rapidity (the linear systems are solved on a plane-by-plane basis and not on a global one, thus diminishing vector performance).

Conclusions

In the present work an efficient and robust computational method for the numerical integration of the compressible Navier-Stokes equations with near-wall k - ϵ closure was developed. The method has optimal convergence (for all of the cases studied) at CFL = 50 and runs from a simple automatic initialization of the flowfield. The time steps obtained are quite large compared with the state of the

art of time-marching schemes using k - ϵ closure for transonic flows. The code is written in SI units.

The results obtained are typical of the near-wall k - ϵ closure. Nonetheless the three-dimensional computations of the Délery B test case highlight a particularly important and usually neglected feature of nominally two-dimensional transonic shock-wave/boundary-layer experiments, i.e., that they are really three dimensional and should be used for code validation as such. Although, because of the inaccuracy of the k - ϵ closure, the agreement of the three-dimensional computations with experiment is not quite satisfactory, the difference between two- and three-dimensional results, obtained by the same code on the same grid, underlines the importance of three-dimensional effects in this case and raises the question of validity of two-dimensional computations that would accurately reproduce this flow. This does not negate the importance of such experiments: it is simply necessary to compute the full three-dimensional configuration.

The satisfactory results for the Délery three-dimensional case are mainly because of the simulation of the second throat. This is very important because there exists no plane before the throat where static pressure is nearly homogeneous.

A grid refinement study has confirmed that n_w^+ is the single most important parameter for accuracy (for transonic flows it is necessary that $n_w^+ \leq 0.75$). In general, lower n_w^+ corresponds to lower computed viscous losses and, as a consequence, a more downstream position of the shock wave. This study has shown that the concept of grid convergence index is not applicable in the case of grids dependent on two parameters, the number of points and the size of the first cell nearest the wall n_w^+ .

The authors are working on many improvements. In order of importance the improvements are improvement of the turbulence model using full Reynolds-stress near-wall closures; the use of accurate Jacobians for the viscous fluxes and eventually of nonfactored implicit schemes, although these would only become competitive for optimal CFL > 500 and can only be implemented in large-memory systems (for the three-dimensional grids used in this study); and the improvement of the space discretization using advanced upwind techniques.

Acknowledgments

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