SPECTRAL ELEMENT SIMULATIONS OF LAMINAR AND TURBULENT FLOWS IN COMPLEX GEOMETRIES

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Spectral element methods are high-order weighted residual techniques based on spectral expansions of variables and geometry for the Navier–Stokes and transport equations. Their success in the recent past in simulating flows of industrial complexity derives from the flexibility of the method to accurately represent nontrivial geometries while preserving the good resolution properties of the spectral methods. In this paper, we review some of the main ideas of the method with emphasis placed on implementation and data management. These issues need special attention in order to make the method efficient in practice, especially in view of the fact that high computing cost as well as strenuous storage requirements have been a major drawback of high-order methods in the past. Several unsteady, laminar complex flows are simulated, and a direct simulation of turbulent channel flow is presented, for the first time, using spectral element techniques.

1. Introduction

Spectral methods have proven in recent years a very powerful tool for analyzing fluid flows and have been used almost exclusively in direct simulations of transitional and turbulent flows [8]. To date, however, only simple geometry turbulent flows have been studied accurately [14], chiefly because of the poor performance of global spectral methods in representing more complex geometries. The development of the spectral element method [26] and its success to accurately simulate highly unsteady, two-dimensional laminar flows [6,13] suggests that a three-dimensional implementation may be the right approach to direct simulations of turbulent flows in truly complex geometries.

There have been several attempts over the past decade to extend the applicability of spectral methods in nontrivial geometries; the approaches followed fall roughly into two categories: The first category consists of all spectral collocation domain decomposition methods that are essentially different extensions of the technique originally proposed by Orszag [22]; the second category consists of variational methods, a successful representative of which is the spectral element method, first suggested by Patera [26]. The primary difference between the patching technique and the variational approach is the treatment of the interfacial continuity condition, which is the most crucial aspect of any domain decomposition method. The extent to which continuity is required at subdomain interfaces would greatly influence the accuracy as well as the simplicity with which the technique can be efficiently implemented. The patching approach is usually associated with spectral collocation methods according to which a differential equation

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of order \( p \) would require the solution and all its derivatives up to order \( (p-1) \) to be continuous along all interfacial collocation points. This interfacial constraint may result in global system matrices that are difficult to invert, in particular in higher dimensions. Moreover, these methods can produce local disturbances near the interface for marginal resolutions resulting in nonconverged solutions [2]. A relatively more efficient approach has been adopted by Macaraeg and Streett [16], where the interface condition is obtained by balancing fluxes globally across the subdomain interfaces.

The spectral element method is a variational domain decomposition technique. The computational domain is broken up into macro-elements within which \textit{variables and geometry} are represented as high-order tensor product polynomial expansions. In the spectral element method mixed collocation variational operators are used to generate the discrete equations with interfacial continuity constraints imposed naturally via the variational statement. This approach results in a weak coupling between dependent variables for adjacent elements and thus symmetric, relatively sparse assembled matrices. The latter is critical as regards the computational complexity of the method in terms of memory requirements and processing time. In addition, the intrinsic "domain decomposition" granularity of spectral element methods leads to natural and efficient implementation on medium-grained parallel processors as explained in detail in [4,5].

The recent advent of parallel processors and appropriate computer solvers have motivated some interesting domain decomposition schemes (which may fall into either of the above categories), such as the alternating Schwarz algorithm, practised in the context of spectral methods by Morchoisne [20]; this technique is a an overlapping domain decomposition method. Along the same lines a relaxation procedure has recently been suggested in [30], where an attempt is made to bypass the construction of global system matrices by solving iteratively a sequence of Dirichlet or Neumann problems for each individual subdomain.

The distinction between the aforementioned two categories has of course its origin in the form of projection operators employed and the associated test functions used. In the first category translated Dirac functions serve as the test functions (collocation scheme), whereas in the second category the basis is also the set of test functions (Galerkin formulation). If exact numerical quadratures are used for the evaluation of integrals involved in the Galerkin formulation it is trivial to show, at least for one-dimensional problems, that the collocation and the variational formulations lead to identical results in the interior of the subdomains [17]. To obtain an exact equivalence among the two formulations the flux condition, which appears as a natural boundary condition in the latter formulation, should explicitly be stated for the former approach. Such an equivalence gives rise to a sort of duality principle for domain decomposition spectral approximation, as pointed out in [2], where it is demonstrated that the variational approximation method can be thought of as a modified patching collocation method.

In this paper we focus on some practical aspects of the spectral element methods and their efficient implementation, and we present several examples of flows in truly complex geometries. In Section 2 the spectral element discretization for Navier–Stokes equations is introduced, and convergence of the method is discussed. In Section 3, an efficient data management scheme is discussed in the context of parallel processing computations. Lastly, in Section 4 we, first, validate the method by comparing the spectral element solutions with the exact eigensolutions of the Orr–Sommerfeld equations in two and three dimensions. In Section 4.2 we present computer-aided flow visualizations for an impulsive flow past a sharp edge wedge; in Section 4.3 we study three-dimensional states of channel flow disrupted by an array of cylindrical eddy
promoters, and finally in Section 4.4 we present the results of a direct simulation of the turbulent flow in a plane channel.

2. Mathematical formulation

We consider here Newtonian, incompressible flows with constant properties, which are governed by the Navier-Stokes equations written in the following form,

\[ \frac{\partial \mathbf{v}}{\partial t} + \nabla \Pi = \mathbf{v} \times \omega + R^{-1} \nabla^2 \mathbf{v} + \mathbf{f} \quad \text{in } \Omega, \]

\[ \nabla \cdot \mathbf{v} = 0 \quad \text{in } \Omega \]

where \( \mathbf{v} = u \mathbf{e}_x + v \mathbf{e}_y + w \mathbf{e}_z \) is the velocity, \( \omega = \nabla \times \mathbf{v} \) is the vorticity, \( \Pi = \rho + \frac{1}{2} \mathbf{v} \cdot \mathbf{v} \) is the pressure head, with \( \rho \) the pressure, and \( R \) is the Reynolds number defined separately for each of the problems we study in Section 4.

The boundary conditions are Dirichlet on moving or rigid walls, Neumann conditions on outflow, and periodicity in homogeneous directions. For purposes of illustration we consider here a model problem with a geometry shown in Fig. 1. The main assumption is that the geometry is homogeneous in the \( z \)-direction, and thus the velocity field as well as the pressure can be decomposed into \( M_z \) Fourier modes in that direction. The dependent variables can then be represented as follows,

\[
\begin{align*}
\mathbf{v}(x, y, z, t) &= \begin{bmatrix} u_{m_z}(x, y, t) \\ v_{m_z}(x, y, t) \\ w_{m_z}(x, y, t) \\ \Pi_{m_z}(x, y, t) \end{bmatrix} \\
\mathbf{v}(x, y, z, t) &= \sum_{m_z=0}^{M_z-1} e^{i \beta m_z z} \\
\end{align*}
\]

where \( \beta = 2\pi/L_z \) is the wave number associated with the homogeneous direction \( z \), and \( L_z \) is

![Fig. 1. Three-dimensional spectral element Fourier computational domain; the geometry is homogeneous and infinite in the \( z \)-direction.](image)
the periodicity length. Typically, $\beta$ is indirectly chosen on the basis of two-point correlation estimates. In the continuous case $M_z \to \infty$, while in the discrete case $M_z$ has a finite integral value.

2.1. Temporal discretization

To solve numerically the above system (1)-(2) we first proceed with the temporal discretization of the equations. Many different approaches can be followed which would lead to different reduced systems of equations; several of the most frequently used schemes are discussed in [23]. An attractive time discretization scheme, particularly due to its ease of implementation in complex geometries, is the multi-fractional step method. This approach was, first, followed by Orszag and Kells [24] for simulating transition to turbulence in a plane channel. In particular, in view of the fact that we seek to simulate high Reynolds number flows, the splitting errors (scaled as $O(\Delta t/R)_{1/2}$) that have been reported in the past to possibly contaminate the solution [18] are negligible for these applications. A fractional step leads advantageously to a decoupled system of Helmholtz operators. We can therefore write the three main substeps as follows:

\[
\begin{align*}
\frac{\hat{v} - v^n}{\Delta t} &= \sum_{q=0}^{2} \beta_q (v \times \omega)^{n-q} & \text{in } \Omega, \\
\frac{\hat{\Phi} - \Phi}{\Delta t} &= -\nabla \Pi & \text{in } \Omega, \\
\hat{\Phi} \cdot \hat{n} &= 0 & \text{on } \partial \Omega, \\
\nabla \cdot \hat{\Phi} &= 0 & \text{in } \Omega, \\
\frac{v^{n+1} - \hat{v}}{\Delta t} &= \frac{1}{2} R^{-1} \nabla^2 \left( \frac{v^{n+1} + v^n}{\Delta t} \right) & \text{in } \Omega, \\
v^{n+1} &= v_w & \text{on } \partial \Omega.
\end{align*}
\]

Equation (4) represents the explicit treatment of the advection terms, where the $\beta_q$ are third-order Adams–Bashforth coefficients: $\beta_0 = \frac{33}{12}$, $\beta_1 = -\frac{16}{12}$, and $\beta_2 = \frac{5}{12}$. We choose the Adams–Bashforth third-order method due to its very low dispersion errors and the relatively large portion of the imaginary axis included within the absolute stability region of the scheme. Equations (5)-(7) represent implicit treatment of the pressure and viscous terms; such an approach results in an efficient and robust inversion of the global system matrices. The time step is therefore dictated by equation (4) and time accuracy considerations. For high Reynolds number flows an explicit treatment of the viscous terms, instead of equation (6), can be followed, since stability constraints due to diffusive contributions are no more stringent than constraints due to the advection contributions. It is the latter approach that we are currently pursuing as it results in significant time savings.

If we now substitute the expressions (3) in (4)-(7) and follow a Galerkin approach in the $z$-direction we obtain the following equations for each mode $m_z$,

\[
\begin{align*}
\frac{\hat{v}_{m_z} - v_{m_z}^n}{\Delta t} &= \sum_{q=0}^{2} \beta_q (v \times \omega)^{n-q} & \text{in } \Omega, \\
\frac{\hat{\Phi}_{m_z} - \Phi_{m_z}}{\Delta t} &= -\nabla \Pi_{m_z} & \text{in } \Omega,
\end{align*}
\]
where in (8) * represents a Fourier transform of the right-hand side of the nonlinear terms. For reasons of efficiency the vorticity \( \omega \) is evaluated in the Fourier space while the nonlinear terms are computed in the physical space before the Fourier transform is performed.

The computation of the pressure in (9) is required as part of the time advancement procedure; the Neumann boundary condition imposed on the pressure is the appropriate one for high Reynolds number flows as is suggested in [23]. We can then easily recast the pressure equation in the following form by incorporating the incompressibility constraint,

\[
\frac{\partial \hat{u}_{m_z}}{\partial x} + \frac{\partial \hat{v}_{m_z}}{\partial y} + i \beta m_z \hat{w}_{m_z} = 0,
\]

where in (8) * represents a Fourier transform of the right-hand side of the nonlinear terms. For reasons of efficiency the vorticity \( \omega \) is evaluated in the Fourier space while the nonlinear terms are computed in the physical space before the Fourier transform is performed.

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following the suggestions by Zang [36], who has found that aliasing errors are much less severe in the latter case.

As regards the spatial discretization of equations (9)–(10) one needs only consider a Helmholtz operator of the form,

\[(\nabla^2 - \lambda^2)\phi = g\] (15)

subject to (for simplicity) homogeneous boundary conditions,

\[\phi = 0 \text{ on } \partial \Omega.\] (16)

If we define \(H^1_0(\Omega)\) to be the Sobolev space for which all the functions vanish at the boundary \(\partial \Omega\), then the variational statement equivalent to (15)–(16) is:

Find \(\phi \in H^1_0(\Omega)\) such that

\[-\int_{\Omega} \nabla \phi \cdot \nabla \psi \, dx - \lambda^2 \int_{\Omega} \phi \psi \, dx \quad \forall \psi \in H^1_0(\Omega).\] (17)

This equation has been studied in detail in [11,15,17] in two and three dimensions, so that only the main points will be reviewed here. In two-dimensional geometries the computational domain is first covered by general, curvilinear quadrilaterals, which are then mapped isoparametrically into locally defined standard finite-like elements, termed hereafter “spectral elements” [15]. Within these mapped squares, independent and dependent variables are expanded in terms of tensor products, for example,

\[\{x, v, \Pi\} = \sum' k \sum_{i=0}^{N} \sum_{j=0}^{N} \{x, v, \Pi\}^k_i h_i(r) h_j(s).\] (18)

where \(\sum'\) represents the coupling between all elements \(k\) (by direct stiffness); here \((r, z)\) defines a local coordinate system, and \(h_i(r), h_j(s)\) are local Lagrangian interpolants of order \(N\), defined as \(h_i(z_j) = \delta_{ij}\), where \(\delta_{ij}\) is the Kronecker delta. This set of interpolants forms naturally the basis with respect to which data and unknowns are expanded in tensor product form as in (18). Such a construction of the solution or the data automatically ensures that both the mapping and the interpolant are in space \(H^1\), a requirement for the variational approach followed to satisfy (15)–(16). The choice of collocation points is, of course, a key factor in achieving high-order accuracy. In the early formulation of the method the Gauss–Lobatto–Chebyshev points were used as local and physical collocation points [26], mainly due to closed form analytical expressions for the quadratures involved in the computation and the possibility of using fast Fourier transforms. However, in recent implementations [17,31], Gauss–Lobatto–Legendre points have been found to be a better choice with all quadratures exactly performed numerically using Gauss–Lobatto integration schemes. In this paper we follow the formulation developed in [15], to which we refer the reader for details. Using the expansions in (18) and substituting into (17) we obtain the discrete elemental equations for the Helmholtz operator,

\[(A^k_{ijmn} - \lambda^2 \hat{B}^k_{ijmn})\phi_{mn}^k = \hat{B}^k_{ijmn} g_{mn}^k,\] (19)

where \(A^k_{ijmn}\) is the stiffness matrix and \(\hat{B}^k_{ijmn}\) denotes the mass matrix. In terms of the discrete
gradient operator $\hat{\nabla}^k$ the above matrices are defined as follows,

\begin{align}
A^k_{ijmn} &= -\hat{\nabla}^k_{pqij} \cdot \hat{B}^k_{pqr} \cdot \hat{\nabla}^k_{rsimn}, \\
\hat{B}^k_{ijmn} &= |J^k_{pq}| \mathcal{B}_{pim} \mathcal{B}_{qjn}, \\
\hat{B}^k_{ijmn} &= |J^k_{pq}|^{-1} \mathcal{B}_{pim} \mathcal{B}_{qjn},
\end{align}

(20) (21) (22)

where $\mathcal{B}$ denotes a local matrix associated with the interpolants as follows,

\begin{align}
\mathcal{B}_{ijk} &= \int_{-1}^{1} h_i(z) h_j(z) h_k(z) \, dz
\end{align}

(23)

and $J^k$ is the Jacobian operator for the isoparametric mapping. The interpolants $h_i$ are computed in closed form in terms of Chebyshev polynomials as explained in [26]. To complete the model problem statement, however, a global assembly of the elemental equations is required, which is done following standard direct stiffness summation. The global system to be solved is,

\begin{align}
L_m \cdot (A^k_{ijmn} - \lambda^2 \hat{B}^k_{ijmn}) Y_{m} &= E^k_{jmn} \mathcal{B}_{mn},
\end{align}

(24)

The set of equations for each Fourier mode $m_z$ resulting from (10) for the computation of the viscous corrections, very closely resembles the above model system of equations. The nonhomogeneous boundary conditions are easily incorporated as part of the solution procedure (Section 3). The equation for the pressure, however, although elliptic in its form, has some unique features that we emphasize next.

2.3. Discrete pressure equation

The pressure equation (13) derived from the semidiscrete treatment of the Navier–Stokes equations deserves special attention, since it involves the incompressibility constraint expressed by (5c). We start by applying the $\nabla \cdot$ operator on both sides of (5a):

\begin{align}
\nabla \cdot \hat{\theta} - \nabla \cdot \hat{\theta} &= -\Delta t \nabla^2 \Pi.
\end{align}

(25)

We can then state the variational analog of the above expression for an appropriate test function $\psi \in H^1$, as follows,

\begin{align}
\int_{\Omega} \psi \nabla \cdot \hat{\theta} \, dx - \int_{\Omega} \psi \nabla \cdot \hat{\theta} \, dx &= -\Delta t \int_{\Omega} \psi \nabla^2 \Pi \, dx.
\end{align}

(26)

The first integral in (26) is zero due to incompressibility constraint from (5c), and thus by integrating both sides by parts we obtain,

\begin{align}
\int_{\Omega} \nabla \cdot (\psi \hat{\theta}) \, dx - \int_{\Omega} \nabla \psi \cdot \hat{\theta} \, dx &= \Delta t \left( \int_{\Omega} \nabla \cdot (\psi \nabla \Pi) \, dx - \int_{\Omega} \nabla \Pi \nabla \psi \, dx \right).
\end{align}

(27)

We can proceed by applying the Gauss theorem on the first terms of both sides of this equation as follows,

\begin{align}
\int_{\partial \Omega} \psi \n \cdot \hat{n} \, dx - \int_{\Omega} \nabla \psi \cdot \hat{\theta} \, dx &= \Delta t \left( \int_{\partial \Omega} \psi \nabla \Pi \cdot \hat{n} \, dx - \int_{\Omega} \nabla \Pi \nabla \psi \, dx \right).
\end{align}

(28)
We can now incorporate the boundary conditions (5a)-(5b), so that the final form of the variational statement for the pressure equation with the Neumann boundary condition for the pressure included as a natural boundary condition is reduced to

$$
\int_{\Omega} \nabla \psi \cdot \hat{e} \, d x = \Delta t \int_{\Omega} \nabla \Pi \nabla \psi \, d x.
$$

(29)

The discrete analog of the above equation can now easily be constructed in terms of the discrete operators introduced in (21)-(23) for each mode $m_z$, as

$$
\sum_k \left( - \tilde{\nabla}^k \nabla \cdot \tilde{B}^k_{pqrs} \tilde{\nabla}^k \Pi_{rmn} - m_z^2 \beta^2 \delta^k_{ijmn} \right) \Pi_{m} = \sum_k \left( - \tilde{\nabla}^k \nabla \cdot \tilde{B}^k_{pqmn} : (\hat{u}_{m, mn} \hat{e} + \hat{v}_{m, mn} \hat{v}) + (i \beta m_z) \hat{B}^k_{ijmn} \hat{\psi}_{m, mn} \right),
$$

(30)

where $\hat{B}^k_{ijmn}$ is a “modified” mass matrix resulting from explicit cancellation of Jacobian terms in the weighted residual formulation and is defined as,

$$
\hat{B}^k_{ijmn} = \text{sgn}(J^k) \int_{-1}^{1} h_i(z) h_m(z) \, dz \int_{-1}^{1} h_j(z) h_n(z) \, dz.
$$

(31)

The discrete equation for the pressure although singular for the mean flow, $m_z = 0$, is always solvable as it is shown in [15]. The only singular mode that appears in the system ($m_z = 0$) is a physical mode (“hydrostatic”) associated with the incompressibility condition. There are no other “spurious” pressure modes, as is typically the case for isoparametric formulations in which velocity and pressure are represented with the same-order interpolants. The fractional formulation results in an elliptic equation for the pressure (29). It is therefore easy, using the ellipticity property of the pressure operator, to prove the uniqueness of the solution for the pressure [13]. Notice that in a coupled pressure-velocity formulation (e.g. the Uzawa algorithm) uniqueness of the pressure solution is not guaranteed, unless appropriate spaces for pressure and velocity fields are selected, [17]. Extensive numerical investigation, especially for stagnation-like flows which have been found to exhibit additional “checkerboard” modes using finite element formulations (Periaux, private communications, [33]), has shown that this is not the case with our system. The success of the pressure step is primarily due to the use of the conservative transpose gradient operator, $\nabla^T$, and the weak imposition of the incompressibility constraint.

Solution of the pressure equation is required as part of the time advancement procedure. The intermediate velocity field $\hat{v}$ can then be determined by collocation as follows,

$$
\left( \hat{u}_{m, ij} - \hat{u}_{m, ij} \right) / \Delta t = - \left( 1 / J^k_{ij} \right) \nabla \hat{\Pi}_{m, mn},
$$

(32)

where $u$ represents the two-dimensional field $(u \hat{e} + v \hat{v})$, with $\circ$ denoting simple collocation product; the equation for the homogeneous component of the velocity field is determined from,

$$
\left( \hat{w}_{m, ij} - \hat{w}_{m, ij} \right) / \Delta t = - (i \beta m_z) \Pi_{m, ij}.
$$

(33)

It is this intermediate field that acts as a forcing for the computation of the final velocity field in (10).
2.4. Convergence rate of the method

We discuss here only the convergence in space of the spectral element method, as the time advancement scheme is a relatively "mature" concept and a complete analysis is given in [23]. The main contributions of the error in the spatial discretization come from the fact that the test functions \( \psi \) that are employed for obtaining the discrete equations belong to a restricted subspace of the space \( H^1 \). Secondly, errors may be introduced by inexact representation of the integrals involved and the insufficiency of the quadrature rules used. As regards the latter, it is the choice of the collocation points that greatly influence this error component. The set of polynomials used in spectral element methods (Chebyshev or Legendre) allows for exact quadrature evaluation with a straightforward implementation. As regards the first error component, there are two different approaches on projecting closer the restricted subspace onto the space \( H^1 \), and thus attain convergence: either the order of interpolants, \( N \), can be kept constant and increase the number of spectral elements, or maintain the number of elements constant and increase the number of collocation points per element. These two different approaches do in fact reflect the difference in convergence "philosophy" between finite element and spectral methods, and in that respect the spectral element method is similar to the \( h-p \) method proposed by Babuška [7]. The convergence rate obtained with the first \( (h\text{-type}) \) approach is algebraic, whereas the convergence rate obtained following the second route \( (p\text{-type}) \) is exponential [26].

Although in the past only numerical evidence existed to support exponential convergence of the method [26], there have recently been obtained rigorous theoretical estimates of error in terms of the best fit of the solution and the forcing. For rectilinear elements the following relationship holds for the continuous solution \( u \) [17]:

\[
\| u - u_h \|_1 \leq C \left( N^{1-\sigma} \| u \|_{\sigma} + N^{(1/2)-\rho} \| g \|_{\rho} \right),
\]

where \( \sigma \) is associated with the degree of smoothness of the solution \( u \) (i.e., \( u \in H^\sigma \)), \( u_h \) represents the discrete solution, and \( \rho \) is the degree of smoothness of the forcing \( g \). The parameter \( C \) is a constant independent of the resolution \( N \). Theoretical error bounds for curvilinear elements is currently a topic of investigation.

Numerical experiments for truly complex geometries for a Stokes problem [15] have demonstrated that exponential convergence is also obtained in this case. Experimentation with the full Navier-Stokes equations using Legendre polynomial expansions accuracy is preserved in the spectral element method.

We conclude this section by commenting on the flexibility of the spectral element method for representing not only curvilinear smooth geometries, but also for treating singular sharp-edge-like geometries. To demonstrate this we solve the Poisson equation in the domain shown in Fig. 2 (A and C) using two different discretization approaches. In both cases a standard isoparametric mapping is employed, according to which the geometry is represented in terms of the same basis as the solution itself (see (18)). The following Poisson equation [31]

\[
\nabla^2 u = 0
\]

is solved, which has the exact (smooth) solution

\[
u = e^{-r} \sin x.
\]

First, the solution is obtained for discretization (A); in this case the geometrical irregularity is
treated as in global spectral methods. This results in poor convergence, as is indicated in Fig. 2, where we plot the error as a function of the total number of degrees of freedom in the x-direction $N_x$. It is seen that the geometrical singularity results in a loss of exponential convergence. The spectral element method, however, offers other alternatives by discretizing the geometry as in (C) shown in Fig. 2. The spectral accuracy is recovered if an elemental interface passes exactly through the sharp corner. For reference, we also include the results of the solution of the same equation solved in the curvilinear domain (B). The exponential convergence is recovered again for the “new” smooth geometry.

3. Data management and implementation

High-order methods, as is the one presented here, are of little practical importance unless efficient algorithmic schemes are employed to solve the global system of equations of the form (13) or (14). There have been numerous approaches proposed for solution of these equations broadly categorized in iterative or direct algorithms. The iterative approach is certainly the only viable one for dynamically deformed geometries or nonconstant property flows. For fixed geometry, however, and constant property flows the direct approach is the best alternative as it is very general and robust; besides, the system matrices need only be inverted once, stored, and retrieved during the time stepping. It is the latter approach that we have been mostly practising to date. In particular, we can apply the standard static condensation algorithm, grouping the nodes and corresponding degrees of freedom into those lying on boundaries of spectral elements, $[\phi^b]$, and those located in the interior of elements, $[\phi^i]$. This practice has been extensively used in the past in finite element methods [34]. The advantage of using static condensation in our method is obvious, since the majority of the nodes is in the element’s interior, with no coupling
between adjacent elemental interior nodes; this latter feature suggests that the major computational work (associated mostly with elliptic solves) can be done in parallel.

The decomposed equations for one element can therefore be written in matrix form as

\[
\begin{bmatrix}
[a^k] & [b^k]^T \\
[b^k] & [c^k]
\end{bmatrix}
\begin{bmatrix}
[b^k] \\
[i^k]
\end{bmatrix}
= \begin{bmatrix}
[b^k] \\
[i^k]
\end{bmatrix}
\begin{bmatrix}
[g^k] \\
[h^k]
\end{bmatrix}.
\]

(36)

Solving separately now for the boundary nodes first, we obtain

\[
\sum_k \left( ([a^k] - [b^k]^T[c^k]^{-1}[b^k])\right)[b^k] = \sum_k \left( [b^k]^T[c^k]^{-1}[i^k]ight).
\]

(37)

The equations for the interior modes can be handled separately for each element after the elemental boundary unknowns have been obtained as follows;

\[
[c^k][i^k] = [g^k] - [b^k]^T[b^k].
\]

(38)

The inversion of the global system matrix in (37) is performed using standard \(LDL^T\) decomposition only once at a preprocessing stage, before the time stepping begins. Thereafter, at each time step only the required forward and backward solutions and matrix multiplications are carried out. For each Fourier mode \(m\), the amount of computational work as operation count per time step is approximately \(O(K^2N^2)\) for the system (37), while for the interior nodes the work is \(O(K^2N^4)\), where each Fourier mode can be thought of as an \(x\)-\(y\) plane discretized in \(K \times K\) elements, each of resolution \(N \times N\). Applying parallel static condensation, however, on a \((K \times K)\)-processor-headed machine the operation count can be reduced to \(O(K^2N^2)\) for the system (37), and to \(O(N^4)\) for the uncoupled system (38).

Our primary interest is in the solution of the time-dependent Navier–Stokes equations at high Reynolds numbers. This would of course require not only an efficient way of solving the system of equations as we described above, but also an intelligent way of managing the large volume of data for problems of industrial complexity. Typically, the amount of data involved is much larger than will fit in the central memory of machines like CRAY-XMP, and thus it is necessary to maintain the data on external storage devices. As the computation proceeds a selective loading of small pieces of data into central memory is also performed. Typically, such devices are available on CRAY environments, called Solid State Devices (SSD). In addition, depending on the demands of the problem, the data can be packed and stored in 32-bit words without effecting the accuracy of the computation.

An efficient data management scheme would require a careful structuring of databases. Our approach is very similar to the one suggested by Kim et al. [14]. As it is shown in the flow chart in Fig. 3, for each time step two passes are taken managing different sections of the databases. This approach is compatible with the fractional stepping method, where the nonlinear terms are decoupled from the two next substeps. In the first pass, PASS1, therefore, the nonlinear terms are computed in the rotational form \(v \times \omega\). At this pass no decoupling between the modes exists and thus all data associated with the \(z\)-direction should be retrieved and loaded in central memory; however this can be done by grouping data for each element (or group of elements) and thus form naturally databases. Notice that at this substep no coupling between elements exists if all required derivatives for the computation of vorticity \(\omega\) have been precomputed and stored. In the second pass, PASS2, the pressure equation as well as the equations for the viscous corrections
are solved. In this pass there is no coupling between the different modes and thus the data that are needed for the elliptic solutions of the form (24) are in x-y planes; the data on these planes, therefore, form now naturally the new databases. Before leaving PASS2, one more step is taken on computing globally the derivatives, which are needed for the following time step in PASS1.

The above data management scheme, besides reducing greatly the storage requirements at essentially no communication cost, is also a scheme highly amenable to parallel processing. As we show in the flow chart in Fig. 3, a number of processors can simultaneously perform computations using z-drawers, say, in PASS1, or using x-y-drawers in PASS2. While computations are carried out in one pass, all communications can be handled at the same time by an independent processor ("manager"). In terms of implementation an efficient and flexible code can be produced by programming the above algorithm in VECTORAL language [35].

4. Numerical simulations

4.1. Two- and three-dimensional Tollmien–Schlichting waves

The Tollmien–Schlichting waves are the viscous solutions of the linearized Navier–Stokes equations (Orr–Sommerfeld equation), describing two- or three-dimensional perturbations of a basic state corresponding to parabolic profile for plane channel flows. Accurate solutions of the Orr–Sommerfeld equations employing eigenvalue solvers have been obtained by Orszag [21]. To examine the accuracy of our code we compute the evolution in time of such small-amplitude waves in a channel. We first test two-dimensional growing waves at Reynolds number $R = 7500$, and streamwise wave number of $\alpha = 1.0$. Here, we nondimensionalize lengths with respect to the half-height of the channel and velocities with respect to the centerline velocity. The channel is discretized with four elements in the streamwise direction and six elements across; each element corresponds to eighth-order Chebyshev polynomials in each direction. The time step was chosen sufficiently small, $\Delta t = 6.3 \times 10^{-3}$, to eliminate time differencing errors. The predicted growth rate, computed from the value of perturbation energy at the critical layer using our initial value...
Fig. 4. (a) A two-dimensional projection of the perturbation field at $R = 1500$, $\alpha = 1.0$. (b) Decay rate versus time at $R = 1500$ and $\alpha = 1.0$.

solvers at two successive time instants, is $\sigma_i = 2.23512634 \times 10^{-3}$ to within $10^{-4}$ percent of the eigenvalue $\sigma_g = 2.23497564 \times 10^{-3}$.

A similar test was performed for a three-dimensional (decaying) wave for $R = 1500$, and stream- and spanwise numbers of $\alpha = 0.5$ and $\beta = 1.0$ respectively. Comparison was made with the independently computed eigenvalue $\sigma_g = -2.400794 \times 10^{-2}$. The decay rate predicted using our initial value solvers was, again, to within $10^{-4}$ percent of $\sigma_g$. In Fig. 4(a) a two-dimensional projection of the velocity field, $v = u\hat{x} + v\hat{y} + w\hat{z}$, is plotted. It is seen that the very thin boundary layers as well as the critical layers located close to the wall (wall modes) are accurately resolved.

An interesting behaviour of our initial value solvers, associated with the fractional time stepping, was observed during those tests. In Fig. 4(b) we plot the decay rate as a function of time; notice that initially there is an overshooting of the decay rate $\sigma_i$, at least for the first few time steps, and asymptotically $\sigma_i$ approaches the eigenvalue $\sigma_g$. This effect is typical of splitting schemes, and it is more pronounced for the $y$-component that is perpendicular to the walls.

4.2. Impulsive flow past a wedge

As our second example, we demonstrate the capability of spectral element methods of representing accurately geometries with sharp corners and obtain high accuracy physical solutions. For this, we consider the flow past a wedge-like sharp edge, as is done in the flow visualization experiment by Pullin and Perry [29]. The wedge is attached to one of the plates of a two-dimensional channel and the flow is started impulsively. A simple, neutrally buoyant dye mixture is injected from both the upstream and downstream faces of the wedge. A two-dimensional vortex ring is formed which grows in time. Instantaneous snapshots of the subsequent motion therefore represent flow streamlines. A number of photographic sequences, for different wedge angles and different starting flows, showing the time-wise primary vortex growth are presented in [29]. The flow past a wedge sharp edge serves as a model for the mechanism of generation of circulation around bodies of aerodynamic interest, and vortex formation understanding is essential in enhancing our knowledge of basic fluid mechanics.

Here, we consider the case of a $\theta = 60^\circ$ wedge angle with an impulsive starting flow. The flow rate is imposed at time $t = 0$ and is set to zero at time $t = 12.52$ s simulating the conditions described in [29, Fig. 5]. In order to visualize the flow in a somewhat analogous manner, we solve...
for a concentration field and the equations of motion simultaneously. Both faces of the wedge maintained at constant concentration level while all other walls are considered impermeable. This approach of computer-aided flow visualizations using scalar transport has been used with success in the past [9] and is expected to produce meaningful results even for this experiment, in which the actual Schmidt number of the dye used in the physical experiment is of the order of thousands; the latter effect seems to be unimportant at least for the initial stages of the vortex ring formation.

In Fig. 5, we present the exact geometry and the spectral element mesh. As regards the geometry, the channel part upstream as well as downstream of the wedge is very close to the dimensions of the apparatus in the physical experiment. A large number of elements has been placed around the wedge and in particular at the wedge tip, where the rolled vortex sheet to be formed emanates; relatively few elements of large dimensions are used in regions where small field gradients are expected. Notice, however, that due to $C^0$ continuity required for the solution and the geometry, only conforming elements can be used. Optimal geometry discretizations are currently under investigation using concepts of nonconforming elements that preserve the spectral accuracy [1,19]. The nonconforming formulation is more general as it couples elements of different order or different number of elements. It is our experience that the discretization presented in Fig. 5 would sufficiently resolve the sharp corner geometrical singularity, as in the case of the singular domain of Fig. 2.

In Figs. 6(a)-(b), we plot a time sequence of concentration contours, during the acceleration phase, while in Fig. 6(c), concentration contours are plotted after the flow is stopped at time $t = 13$ s for Reynolds number $R = 1560$, where $R = Q/\nu$. Here $Q$ is the imposed flow rate, and $\nu$ is the fluid viscosity. These plots show a very close resemblance with the photographs of [29, Fig. 5] although the two flow visualization mechanisms are somewhat different. Not only the computed primary vortex ring is very similar in form and size to the one observed experimentally, but the resemblance extends to secondary flow details, such as the near the wedge-apex separation bubble. In more quantitative form, the horizontal position of the vortex ring center, $x^\nu$ can be used as a measure of comparison. For example, at time $t = 5$ s, the computed $\xi^\nu = 2.50$ cm compares well with the value $\chi^\nu = 2.60$ cm measured in [29]. Our results are much closer to the similarity solutions reported in [28], whereas the experimental results depart
Fig. 6. Concentration contours at (a) $t = 5\, s$, (b) $t = 9\, s$ and (c) $t = 13\, s$. The computer-aided flow visualizations resemble very closely the physical experiments described in [29, Fig. 5].
somewhat from the similarity results for the case we analyze. Finally in Fig. 7 the vortex ring formation process is visualized using fluid markers for instantaneous velocity fields. In these plots some salient details of the flow are revealed, not previously realized by other workers [32]. The main flow features, such as the inviscid rotational primary vortex with its viscous subcore, which have also been identified previously by other workers are present in our simulations. In addition, however, our results indicate that at the tip of the wedge a viscous separation bubble is developed after time $t = 4s$, with two standing vortices formed, and the fluid is locally in countermotion with the primary vortex ring. Details of the flow structure as well as more quantitative measurements of the position of the various eddies can be found in [12].

4.3. Three-dimensional flow in eddy-promoter channels

The two-dimensional flow past an array of cylindrical eddy promoters placed in a periodic fashion in a smooth channel has been studied in detail in [13]. It was shown that the addition of even small cylinders results in excitation of stability modes at relatively low Reynolds numbers, which resemble both in form and frequency to plane channel Tollmien-Schlichting waves. For the standard two-dimensional geometry studied in [13], the (linear) critical Reynolds number was found to be $R_c = 150$, much lower than the critical Reynolds number in plane channels at $R_{cp} = 5772$ [21]. (The Reynolds number, here, is defined based on channel half-height and the centerline velocity.)

In this section we investigate three-dimensional states of this flow; the geometry is of infinite extent in the spanwise direction, and the flow varies along all three directions. The discretization then proceeds by breaking the computational domain in two-dimensional Chebyshev–Chebyshev spectral elements in the $x$-$y$ plane, with $M_z$ Fourier modes employed for the discretization along the homogeneous $z$-direction. It is shown in [10] that wall-bounded flows of the type we study here exhibit similar hydrodynamic stability as the plane Poiseuille flow, with a secondary instability following the first two-dimensional bifurcation [25].

A typical spectral element mesh in the $x$-$y$ plane for this simulation is shown in Fig. 8. The cylinder is located halfway between the wall and the channel centerline, and its diameter is $0.20H$ where $H$ is the channel height. Periodic boundary conditions are employed in both the stream- and spanwise directions.
Typical computations were carried out with $M_z = 4$ and 8 modes in the $z$-direction. The initial conditions correspond to a three-dimensional Tollmien–Schlichting wave. The integration was carried out for long time (500 nondimensional time units), to ensure that the flow achieves an asymptotic state; the time step of the computation was of the order of $\Delta t = 1.0 \times 10^{-2}$. In Fig. 9(a), we plot the instantaneous velocity field at Reynolds number $R = 300$ in plane corresponding to $m_z = 0$, and in Fig. 9(b) we plot the deviation of the velocity field in a plane with index $m_z = 3$. It is shown that at this Reynolds number three-dimensional structures have been formed indicative of a secondary flow of the form described in [25]. The basic two-dimensional oscillatory flow is obtained via a regular Hopf bifurcation caused by the shear layer instability as explained in [13].

4.4. Turbulent flow in a plane channel

As our last example we simulate the flow in a plane channel at Reynolds number $R_s = 100$, where the Reynolds number is based on the shear velocity $U_s$ and the channel half-height, $H$. This inhomogeneous flow has been successfully simulated by spectral codes [14], and excellent agreement for most of the turbulence statistics has been obtained with the experimental data.

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Fig. 8. Spectral element mesh for a flow past an array of eddy promoters. The geometry is assumed to be infinite (periodic) in $x$- and $z$-directions; the flow is allowed to vary in all three directions.

Fig. 9. (a) Instantaneous velocity vectors for flow past an array of eddy promoters at a plane $m_z = 0$ ($R = 300$, $\alpha = 1.0$). (b) Deviation of velocity field from the field described in (a) at a plane $m_z = 3$. Three-dimensional structures develop at this Reynolds number resembling Tollmien–Schlichting waves.
Fig. 10. Spectral element mesh for the simulation of turbulent flow in a channel. The streamwise periodicity length is $L_x = 6\pi H$ and the spanwise periodicity length is $L_z = \frac{3\pi}{2} H$. The minimum spacing in the vertical direction is $y_{\text{min}} = 0.05$ and the maximum is $y_{\text{max}} = 9.5$ wall units.

Fig. 11. Mean velocity profile for turbulent flow in a channel at $R_e = 100$.

Our purpose here is to determine if the spectral element method can sustain turbulence at this marginal Reynolds number; low-order schemes usually fail to maintain the turbulent fluctuations and force the flow to return to laminar state. The initial conditions were obtained using the spectral code of Kim et al. [14] for similar flow conditions.

The computational domain is shown in Fig. 10; the domain is broken up into 24 spectral elements in the $x$-$y$ plane. The local resolution is chosen to be Chebyshev eighth-order polynomials in both $x$- and $y$-directions, while 32 Fourier modes are employed in the $z$-direction with the $z$-collocation points equally spaced. Note that the macro-element discretization was chosen so that the spacing in the $y$-direction matches the spacing of a global spectral discretization employing 33 collocation points across the channel. The minimum $y$-spacing is $\Delta y^+ = 0.05$, and the maximum $y$-spacing is $\Delta y^+ = 9.5$, with respect to wall units. Our discretization in the streamwise direction differs significantly from all past simulations which have employed uniform meshes in both $x$- and $z$-directions. The size of the computational domain is typically guided by two-point correlation estimates using experimental data. This approach has been followed with success in the past by the practitioners of direct simulations of turbulent flows. Typically, for plane channels and for the range of Reynolds number we can currently reliably simulate, velocity fluctuations do not correlate at a distance of $\delta_{x_1} = 1.6 H$ in the streamwise direction and $\delta_{x_3} = 0.8 H$ in the spanwise direction. Computation of energy spectra in those directions after the solution is obtained is usually required to test this assumption. In our simulation the streamwise length is $L_x = 6\pi H$, and the spanwise length is $L_z = \frac{3}{2}\pi H$.

In Fig. 11 we plot the mean velocity profile across the channel for Reynolds number $R_e = 100$. The centerline velocity is $U_{\text{cl}} = 18.2 U_e$ and therefore the Reynolds number $R$ is approximately 1820. This mean profile is reached after integration of the spectral element equations for long time, $O(t) = 5$, starting from the spectral solution of Kim et al. [14]. The time step employed for the time integration was $\Delta t = 1.0 \times 10^{-3}$. The fact that the solution remains unchanged is an indication that the spectral element method can sustain the turbulent fluctuations. Comparison of the mean profile with experimental data gives an excellent agreement [14]. Turbulence intensities $U_{\text{rms}}, V_{\text{rms}}$ and $W_{\text{rms}}$ normalized by the wall shear velocity are shown in Figs. 12(a)–(b).
Fig. 12. (a) Streamwise turbulence intensity for the flow described in Fig. 10. (b) Vertical and spanwise turbulence intensities normalized with the wall shear stress.

The initial and final profile shapes are indistinguishable. Moreover, they are in good agreement with experimental results; similar comparisons are made in [14]. Notice that the slight asymmetry in the \( \nu \)-component is present in the initial data and it is indicative of marginal resolution. In Fig. 13(a) and (b) the Reynolds shear stress and the local correlation coefficient respectively are plotted for the final time. The Reynolds stress is, in particular, a good measure of when a statistically steady state is reached as it balances the induced pressure drop. The near-wall behaviour of the Reynolds stress scales as \(-\bar{u} \bar{v}' \sim y^3\), although this limiting behavior has been the subject of disagreement [3]. However, our results fully agree with the results of Kim et al. [14], which support this conclusion. As regards the correlation coefficient, it differs slightly from the one computed by Kim et al. at \( R_s = 180 \), where a weak peak is present close to the walls indicative of organized motions. It is probably the inadequacy of the resolution in the current simulation very close to the wall that is responsible for this discrepancy.

The above computation was carried out on the CRAY-XMP/48 computer at NASA Ames Research center. The CPU time required for this computation is approximately 7.5 s/\( \Delta t \), with a slight overhead at a preprocessing stage for forming and inverting the global system matrices. This cost seems to be approximately eight times higher than a global spectral simple geometry code (e.g. Kim et al.) for a commensurate number of degrees of freedom that corresponds to only one Chebyshev and two Fourier directions. This computational cost, however, can be reduced by an order of magnitude by exploiting parallel architectures, pertinent to spectral element discreti-
zations (Section 3). Such a formulation of a high efficiency medium-grained parallel spectral element method was implemented recently on the INTEL vector hypercube [4]; the results demonstrate, indeed, the true advantages of parallel spectral element methods. In terms of memory requirements only a fraction (0.8 Mwd) of the available central memory of the CRAY-XMP/48 (8 Mwd) was required, equivalent to memory requirements of codes for applications in simple geometries. These savings are mainly the result of implementing efficiently in VECTRAL language [35] the data management scheme discussed in Section 3. Our formulation is general and applicable to direct simulations of turbulent flows in complex $x$-$y$ geometries that have not been addressed before; such an example is the flow in the geometry in Fig. 1. We are currently investigating turbulence structures in these complex geometry flows.

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