Navier-Stokes solver using Green’s functions II: spectral integration of channel flow and plane Couette flow

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Abstract

The Kleiser-Schumann (1980) and Kim-Moin-Moser (1987) algorithms for solving the incompressible Navier-Stokes equations have been used to simulate a great variety of turbulence phenomena in plane channels and in plane Couette flow. In this article, we derive new versions of either algorithm which completely eliminate numerical differentiation in the wall-normal direction. We argue that the new versions should be able to reach higher Reynolds number than currently possible, thanks to their greater accuracy. Using $10^9$ grid points and only 10 compute nodes, they reach a frictional Reynolds number ($Re_\tau$) of 2380 (with bulk flow $Re = 80,000$), which may be compared with the simulation of Hoyas and Jiménez (2006, 2008) which reached $Re_\tau = 2003$. The methods derived here appear capable of going well beyond $Re_\tau = 2380$.

1 Introduction

The incompressible Navier-Stokes equation $\partial u/\partial t + (u, \nabla) u = -\nabla p + \triangle u/Re$, where $u$ is the velocity field and the pressure $p$ a Lagrange multiplier for enforcing the incompressibility constraint $\nabla \cdot u = 0$, is an adequate physical model for a very great variety of phenomena pertaining to fluid flows. Among these, turbulence is one of the most dramatic. The ability to reproduce this phenomenon in computer simulation has been an aid to progress in this area of science. Turbulence manifests itself at even low Reynolds numbers ($Re$) and becomes more pronounced as $Re$ increases.

The first computer simulation of fully developed turbulence in wall bounded flows was reported in a landmark paper by Kim, Moin, and Moser [7]. Even to this day, the algorithm in that paper and its variations are used by computer simulations that strive to reach higher Reynolds numbers in channels and plane Couette flow. Another effective and widely used algorithm for channel and plane Couette geometries is due to Kleiser and Schumann [8]. In this article, we remove the principal source of rounding error in both the Kleiser-Schumann and Kim-Moin-Moser algorithms.

Both channel and plane Couette geometries are rectangular. In the notation adopted here, the wall-normal axis is $y$ and the $x, z$ axes are parallel to the wall. The velocity field $u$ is assumed to be periodic in the wall-parallel directions with periods equal to $2\pi \Lambda_x$ and $2\pi \Lambda_z$. The walls are assumed to be at $y = \pm 1$. In channel flow, the velocity field $u$ satisfies the boundary conditions $u(x, \pm 1, z) = 0$. The flow is driven either by a constant pressure gradient or by fixing the mass flux. Plane Couette flow is wall-driven and satisfies the boundary conditions...
The velocity field $\mathbf{u} = (u, v, w)$ is represented as

$$\mathbf{u} = \sum_{l=-L/2}^{L/2} \sum_{n=-N/2}^{N/2} \hat{\mathbf{u}}_{l,n}(y) \exp \left( \frac{ilx}{\Lambda_x} + \frac{inz}{\Lambda_z} \right)$$

with $\hat{\mathbf{u}}_{l,n} = (\hat{u}_{l,n}, \hat{v}_{l,n}, \hat{w}_{l,n})$. If either $L$ or $N$ is even, the $\pm L/2$ and $\pm N/2$ terms are collapsed into a single cosine (or set to zero for convenience). The three components of $\hat{\mathbf{u}}_{l,n}$ are represented using Chebyshev polynomials $T_n(y)$ as $c_0/2 + \sum_{j=1}^{M-1} c_j T_j + c_M T_M/2$ (it is typical to set $c_M$ to zero for convenience). The number of grid points in the $y$ direction is always denoted by $M + 1$. This type of representation of velocity fields was first employed by Orszag [12] in 1971. Indeed, this pioneering paper by Orszag introduced the use of Chebyshev series to fluid mechanics and more generally to the solution of partial differential equations. The paper contains a complete method for the solution of the Navier-Stokes equations, which has never been implemented to the best of this author’s knowledge. Although complete, the method appears far too expensive, and even apart from its high cost, its effectiveness or accuracy is hard to assess.

An important step towards an effective and affordable solver was taken by Gottlieb and Orszag [3, p. 119]. They showed how to rewrite the Chebyshev tau equations for solving boundary value solvers of the equation $(D^2 - a^2) u = f(y), u(\pm 1) = 0$, where $D$ denotes $\frac{d}{dy}$, as a tridiagonal matrix with bordered rows. They also remarked that more accurate solutions
could be obtained using the new form of the equations. The improvement to the Kleiser-Schumann and Kim-Moin-Moser algorithms made in the present paper lies in this region. The use of tridiagonal matrices with bordered rows has persisted since the work of Gottlieb and Orszag. We show that the bordered rows can be and ought to be eliminated to derive more robust solvers. The equations of Gottlieb and Orszag are now recognized as a form of spectral integration.

Orszag and Kells [13] derived a Navier-Stokes solver and used it to study transition to turbulence in channels and plane Couette flow. This solver is first order in time, and splits the nonlinear term, the pressure term, and the viscous term into three separate equations. The solution for the pressure term, which enforces the incompressibility condition, uses spectral integration. Another method, which does not rely on splitting, was derived by Orszag and Patera [14].

Another big step towards an effective and affordable solver was taken by Moin and Kim [9]. In that article, the difficulties in handling the pressure term in channel flow are brought to light. Solving the Poisson equation for pressure at every step means that the incompressibility constraint is not being enforced. Instead, the incompressibility condition must be used to solve for pressure. Moin and Kim showed how to obtain block tridiagonal systems to solve for pressure. The handling of the pressure term is explained thoroughly and with wide-ranging context by Rempfer [15].

Kleiser and Schumann [8] realized that the Poisson equation for pressure may be solved for pressure, provided the boundary conditions require incompressibility of the velocity field at the walls. The Kim-Moin-Moser method [7] eliminates pressure completely. As noted by its discoverers, the Kim-Moin-Moser method is similar to the technique in [14]. Implementing these methods poses challenges that go well beyond the algorithms. As far as the comparison of numerical solutions of the Navier-Stokes equations to experiments (and not theory) in the turbulent regime is concerned, there is nothing prior to [7] to the best of this author’s knowledge. In contrast, the comparisons in [7] are detailed and extensive and set the standard for later research.

Both Kleiser-Schumann and Kim-Moin-Moser methods come down to solving boundary value problems of the form \((D^2 - a^2) u = f(y), u(\pm1) = 0\), or its fourth order counterpart \((D^2 - a^2)(D^2 - b^2) u = f(y), u(\pm1) = Du(\pm1) = 0\). Throughout this paper, \(D\) stands for \(\frac{d}{dy}\). There are two difficulties that arise in solving such problems. The first pertains to finite difference or finite element type methods. These methods discretize the derivative directly and the resulting linear systems have condition numbers of \(O(M^2)\) for second order problems and \(O(M^4)\) for fourth order problems, where \(M\) is the number of grid points along \(y\). This phenomenon is well-explained in finite element textbooks, but briefly stated, it arises for the following reason: for an \(m\)-th order problem, eigenmodes that oscillate with spatial period of the order of the grid spacing correspond to eigenvalues that are approximately \(M^m\) times the eigenvalue of the fundamental mode. There is no way around it as long as derivatives are discretized. In fact, it can be much worse than \(O(M^m)\) because the grid must be non-uniform and finer near the walls. For the fourth order problems that arise in the Kleiser-Schumann and Kim-Moin-Moser methods, even \(M = 1000\) is possibly enough to render the calculations too inaccurate to be useful in double precision arithmetic (with \(\epsilon_{machine} \approx 10^{-16}\)).

Fortunately, the bordered tridiagonal systems used to solve for Chebyshev coefficients have never suffered from this instability. The linear systems correspond to spectral integration...
in which the differential operator is analytically inverted to get an integral operator, thus overcoming the condition number. Instead, the main source of error comes in while evaluating the nonlinear term which involves second derivatives in both methods. Since the Chebyshev grid is quadratically clustered at its endpoints, the error in evaluating a second derivative is $O(M^4)$. Once again we are restricted to $M \leq 1000$, but for a different reason.

The two methods derived in this paper eliminate numerical differentiation with respect to $y$ completely. Both are based on [20]. Although spectral integration has been used for a long time, many of its properties were not well understood. In [20], better understanding is attained of several properties of spectral integration. Many new forms of spectral integration are derived. The methods given here combine some of those forms of spectral integration. We do not work with bordered tridiagonal systems but with perfectly tridiagonal systems. The methods are optimally adjusted to the Navier-Stokes equations. While eliminating numerical differentiation in the $y$ direction, these methods ensure no intermediate quantity that is not needed is computed. This implies efficient use of memory, which is of value in large computations. Large computations are chiefly limited by the amount of memory available per node.

One of the largest $Re_\tau$ attained among published calculations appears to be due to Hoyas and Jiménez [4, 5], who have reported simulations at $Re_\tau = 2003$. Hoyas and Jiménez use compact finite differences to discretize derivatives in the $y$ direction. The resulting ill-conditioning is necessarily worse than $O(M^4)$. In fact, the number of grid points along $y$ is given by $M = 632$. Unlike the Chebyshev grid which is quadratically clustered at the endpoints $y = \pm 1$, the Hoyas-Jiménez grid is clustered like the $1.5$-th power at $y = \pm 1$. The rounding error in calculating second derivatives is only of the order $O(M^3)$. The success of compact finite differences shows the value of mitigating errors in numerical differentiation.

In a recent paper, Bernardini and others [1] have reached $Re_\tau = 4000$ using $M = 1024$. The wall-normal spacing $\Delta y^+ = 12.3$ used there is greater than in [4, 5] or Section 5, showing that the main constraints are in the wall-normal direction. The wall-normal grid is not Chebyshev. Time is advanced using a fractional step method. Pressure is coupled to the zero divergence condition in a fractional step method, as it should be, but the coupling with the velocity evolution equations is not maintained. There is a loss in order of accuracy, but no fourth order boundary value problems are solved numerically. For the second order boundary value problems that arise, the ill-conditioning of finite difference matrices is not $O(M^4)$ but the much more manageable $O(M^2)$. The dominant source of rounding error here is due to the second derivative in the wall-normal direction and the clustering of grid points at the boundaries.

State of the art simulations such as [1, 4, 5] have resorted to finite differences for two main reasons. With finite differences, one can choose a wall-normal grid that resolves the flow using about half the number of points of Chebyshev. As an added benefit, the CFL (Courant-Friedrichs-Lewy) condition is eased. Thus the Navier-Stokes equation can be integrated over a longer period using fewer CPU hours. In part III of this sequence, the present paper being part II, we will extend the Green’s function method of part I [21] to the Hoyas-Jiménez grid so as to preserve the chief advantages of finite-difference grids. With regard to Green’s functions, it must be mentioned that some of the calculations in part III will parallel the analysis of pressure fluctuations in a channel by Kim [6]. A complete discussion of that connection will

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1 A careful implementation of Kleiser-Schumann which passes from the velocity field to the vorticity field using Chebyshev coefficients, but not passing to physical space except to evaluate the nonlinear term, can eliminate part of the error in one derivative. See [11]. A fuller description of how this trick works will be given when [20] is revised.
be included in part III.

2 A boundary value solver for \((D^2 - a^2) u = f + \frac{dg}{dy}\)

In this section, we describe a boundary value solver for the linear equation

\[
(D^2 - a^2) u(y) = f(y) + \frac{dg(y)}{dy}, \quad u(1) = A, \ u(-1) = B.
\] (2.1)

This solver is the basis of the new version of the Kleiser-Schumann algorithm given in the next section. The inputs to the solver are the functions \(f(y)\) and \(g(y)\), or the truncated Chebyshev series representing those functions. Its outputs are the function \(u(y)\) and its derivative \(Du(y)\), which are again represented using Chebyshev series. Although \(g(y)\) is differentiated on the right hand side of (2.1) and the solver outputs \(Du\) along with \(u\), the solver does not differentiate numerically. The transformation of inputs to outputs is based on integration of Chebyshev polynomials and the solution of tridiagonal systems.

In [20], two forms of spectral integration are described. Applying the first form to the boundary value problem (2.1) would begin by expanding \(u(y)\) in a Chebyshev series. The second form would begin by expanding \(D^2 u(y)\) in a Chebyshev series. The method given here does neither. Instead \(Du\) is expanded in a Chebyshev series. Doing so leads to a version of the Kleiser-Schumann algorithm that does exactly what is needed to eliminate numerical differentiation but nothing more.

2.1 Spectral integration

The boundary value problem (2.1) is integrated once with respect to \(y\) to get the following equation.

\[
Du - a^2 \int \int Du = \int f + g.
\] (2.2)

The solution derivative \(Du\) is expanded in a truncated Chebyshev series as \(\alpha_0 T_0(y)/2 + \sum_{j=1}^{M-1} \alpha_j T_j(y) + \alpha_M T_M(y)/2\). We use \(T_j(u)\) to denote the coefficient \(\alpha_j\) in the Chebyshev series expansion of \(u(y)\). For convenience, \(T_M(u) = \alpha_M\) is assumed to be zero.

The first step is to find the particular solution of (2.2) subject to the integral conditions \(T_0(u) = T_0(Du) = 0\). Because \(T_0(u) = 0\), there is no indeterminate constant in the Chebyshev series of \(u\) obtained by integrating \(Du\):

\[
u = \int Du = \sum_{j=1}^{M-1} T_j \left( \frac{\alpha_{j-1}}{2j} - \frac{\alpha_{j+1}}{2j} \right)
\] (2.3)

where \(\alpha_0 = \alpha_M = 0\). This equation is integrated once more, once again using \(\int T_n = T_{n+1}/2(n+1) - T_{n-1}/2(n-1)\) for \(n > 1\), \(\int T_1 = T_2/4\), and \(\int T_0 = T_1\), to get

\[
Du - a^2 \int \int u = C + T_1 \left( \alpha_1 + a^2 \left( \frac{\alpha_1}{8} - \frac{\alpha_3}{8} \right) \right) + \sum_{j=2}^{M-1} T_j \left( \alpha_j - a^2 \left( \frac{\alpha_{j-2}}{4j(j-1)} - \frac{\alpha_j}{2(j^2-1)} + \frac{\alpha_{j+2}}{4j(j+1)} \right) \right)
\]
where $\alpha_0 = \alpha_M = \alpha_{M+1} = 0$. Here $C$ is an indeterminate constant.

Similarly, if $T_j(f) = f_j$ and $T_j(g) = g_j$ in the truncated Chebyshev series of the functions $f$ and $g$, the expansion of $\int f + g$ is given by
\[
\int f + g = C + \sum_{j=1}^{M-1} T_j \left( \frac{f_{j-1}}{2} - \frac{f_{j+1}}{2} + g_j \right)
\]
where $C$ is another indeterminate constant and it is assumed that $f_M = g_M = 0$. Equating the Chebyshev coefficients on either of side of (2.2) for $C$ we have
\[
\begin{align*}
(1 + \frac{a^2}{8}) \alpha_1 - \frac{a^2}{8} \alpha_3 &= \frac{f_0}{2} - \frac{f_2}{2} + g_1 \quad \text{for } j = 1, \text{and} \\
-\left(\frac{a^2}{4j(j-1)}\right) \alpha_{j-2} + \left(1 + \frac{a^2}{2(j^2-1)}\right) \alpha_j - \left(\frac{a^2}{4j(j+1)}\right) \alpha_{j+2} &= \frac{f_{j-1}}{2} - \frac{f_{j+1}}{2} + g_j \quad (2.4)
\end{align*}
\]
for $j = 2, 3, \ldots, M-1$. These $M-1$ equations decouple into two tridiagonal systems of dimensions $M-2 + M \mod 2$ and $M-M \mod 2$ for the even and odd modes, respectively. The equations are solved for $\alpha_1, \ldots, \alpha_{M-1}$ to find the Chebyshev series of $Du$. The Chebyshev series of $u$ is found using that of $Du$ (2.3). This particular solution $u$ satisfies the integral conditions $T_0(Du) = T_0(u) = 0$.

The particular solution found in this way is quite inaccurate when $a$ is large, which is the typical situation when the Reynolds number $Re$ is large. However, the boundary value problem (2.1) can still be solved accurately. To do so, the homogeneous solutions of (2.1) must be found in a peculiar way. For reasons explained in [20], this peculiar way of finding homogeneous solutions leads to a cancellation of discretization error and an accurate solution of the original boundary value problem.

One of the homogeneous solutions is taken to be of the form $u_{h1} = \frac{1}{2} + u$ with $u$ satisfying $T_0(Du) = T_0(u) = 0$. Then $u$ satisfies $(D^2 - a^2) u = a^2/2$. Thus $Du_{h1}$ and $u_{h1}$ may be found by solving (2.4) with $g \equiv 0$ and $f_0 = a^2$, $f_1 = \cdots = f_M = 0$.

The other homogeneous solution is taken to be of the form $u_{h2} = T_1/2 + u$ with $T_0(Du) = T_0(u) = 0$ as before. This time $(D^2 - a^2) u = a^2 T_1/2$ and (2.4) must be solved using $f_1 = a^2/2$ and $f_0 = f_2 = \cdots = f_M = 0$.

Finding the particular solution $u$ and the homogeneous solutions $u_{h1}$, $u_{h2}$ involves solving a total of 6 tridiagonal systems each of dimension approximately $M/2$. In the linear combination $u + c_1 u_{h1} + c_2 u_{h2}$ the coefficients $c_1$ and $c_2$ are calculated by setting the boundary values at $\pm 1$ to $A$ and $B$ as in (2.1). The solution derivative is given by $Du + c_1 Du_{h1} + c_2 Du_{h2}$.

Here the derivatives $Du$, $Du_{h1}$, $Du_{h2}$ are from solving the tridiagonal systems and not from numerical differentiation. The function $g(y)$ on the right hand side of (2.1) is not differentiated numerically either.

This method of solving the boundary value problem (2.1) is the one that will be used to make the Kleiser-Schumann algorithm more robust. Here we will describe a more general method. In this more general method, the interval $[-1, 1]$ is broken up into abutting intervals $I_1, \ldots, I_m$. Each one of these intervals is discretized using Chebyshev points. To solve (2.1), a particular solution $u_\mu$ and homogeneous solutions $u_{h1,\mu}$ and $u_{h2,\mu}$ (as well as their derivatives) are calculated over each interval $I_\mu$ with $1 \leq \mu \leq m$. If the linear combination over the interval $I_\mu$ is
\[
u_\mu + c_\mu u_{h1,\mu} + d_\mu u_{h2,\mu} \quad \text{for } 1 \leq \mu \leq m
\]
A boundary value solver for \((D^2 - a^2) u = f + \frac{da}{dy}\)

\[
D^2 - a^2) u = f, u(\pm 1) = 0
\]

the exact solution, plotted against the number of terms in the Chebyshev series. The derivative \(\frac{du}{dy}\) is either calculated using spectral integration as described in the text or by numerically differentiating the calculated \(u\).

then the following equations are used to solve for \(c_\mu\) and \(d_\mu\): the two boundary conditions of \((2.1)\), \(m - 1\) equations for continuity of \(u\) at interval endpoints other than \(\pm 1\), and \(m - 1\) equations for continuity of \(Du\) at the same points. These equations are banded.

This more general method offers the possibility of choosing the abutting intervals \(I_\mu\) to form an outer grid that is clustered like the 1.5-th power at the endpoints as in \([4, 5]\). Good order of accuracy is implied by the inner Chebyshev grid inside each \(I_\mu\). We may hope that turbulent channel flow can be resolved using fewer grid points in the wall-normal direction.

This more general method has been implemented and the hope is not entirely false. However, the inner Chebyshev grid forces very small CFL numbers and time steps making the extra generality of no use.

### 2.2 Numerical properties

The errors in nearly all numerical calculations of solutions of differential equations are discretization errors. Rounding errors too are of course present, but \(\epsilon_{\text{machine}} \approx 10^{-16}\) in IEEE double precision arithmetic is so small that the rounding errors are rarely noticeable. Discretization errors are much better understood. Concepts such as order of accuracy and truncation error bring them under the sway of mathematical reasoning. It is much harder to reason about rounding errors.

As far as the numerical computation of turbulent solutions of the Navier-Stokes equation is concerned, more than two decades of work beginning with \([7]\) has produced an understanding of grid resolutions needed for obtaining reliable results. The grids that are needed to advance computations beyond currently achievable Reynolds numbers are so fine that rounding errors are now the major impediment.

Here we will look at the rounding errors that arise when boundary value problems are
solved using the method described earlier in this section. Figure 2.1a compares the error in the derivative \( du/dy \) obtained as a part of spectral integration with the error in the derivative computed by numerically differentiating \( u \). The numerical differentiation is performed using the discrete cosine and sine transforms (DCT and DST). It is important to note that the numerical differentiation is from physical to physical domain (see [11] and [20]). The error in the numerical derivative grows at a rate that appears slightly worse than quadratic in \( M \), the size of the Chebyshev grid. Quadratic growth of error is expected because the Chebyshev points \( y_j = \cos(j\pi/M) \), \( 0 \leq j \leq M \), are quadratically clustered at \( \pm 1 \). The increase in errors is much milder if the derivative is computed using spectral integration.

The growth of rounding errors is quartic for the 2nd derivative. There can be little doubt that \( M = 10^4 \) would be unachievable if derivatives are computed numerically and that problems will set in even near \( M = 10^3 \). Spectral integration appears to get around this limitation.

It must be noted, however, that Figure 2.1a is much too optimistic with regard to the efficacy of spectral integration. Figure 2.1b shows errors for the same differential equation \( (D^2 - a^2) u = f \) with \( a = 10^6 \) instead of \( a = 10 \). In this instance, the errors in spectral integration increase quadratically with \( M \) (for \( M < 5000 \)) just as for numerical differentiation.

This quadratic increase may be explained as follows. When \( a \) is large, we have \( u \approx -f/a^2 \) away from the boundary layer and \( du/dy \approx -df/dy \times a^{-2} \). Thus taking the derivative of \( u \) is almost equivalent to taking the derivative of \( f \) and there is no trickery that can save us from differentiation errors when the solution operator fails to have a smoothing effect. However, even with \( a = 10^6 \) in Figure 2.1b, it is noticeable that spectral integration still does better. In particular, for \( M \approx 10^4 \) the derivative obtained using spectral integration is better by more than 4 digits. In computing turbulent solutions of channel flow \( a = 10^6 \) would imply \( M \geq 10^4 \).

For the numerical results given in Section 5, \( a \approx 1.7 \times 10^4 \) and the Reynolds number reached is \( Re_f \approx 2380 \) or \( Re = 8 \times 10^4 \). To a first approximation, \( a = (Re/\Delta t)^{1/2} \) where \( \Delta t \) is the time step. It appears that Reynolds numbers that are ten times as high can be reached with \( a \approx 10^5 \). For such \( a \), the gain in accuracy due to spectral integration will be somewhere in-between Figure 2.1a and (b) and may correspond to saving 4 or 5 or 6 digits from rounding errors, which is enough to render the calculations feasible.

In Figure 2.2a, the value of \( a = 2 \times 10^4 \) is close to what occurs in the \( 10^9 \) grid point computation given later. In Figure 2.2b, \( f \) is chosen so that \( u = \sin k\pi y \), with \( k \approx M/6 \), implying approximately 6 points per wavelength. At \( M = 10^3 \), which is the \( M \) in that computation, we see that spectral integration boosts the accuracy of derivatives by slightly less than 3 digits in Figure 2.2a and by slightly more in Figure 2.2b.

To get a sense of how rounding errors influence solutions of the Navier Stokes equations, we may oversimplify and assume that computed solutions are solutions of the perturbed equation

\[
\frac{\partial \mathbf{u}}{\partial t} + \omega \times \mathbf{u} = -\nabla p + \frac{1}{Re} \Delta \mathbf{u} + \text{discretization error} + \text{rounding error}.
\]

Discretization errors get smaller as the computational grid is refined while the rounding errors get larger. The point where rounding errors begin to cause trouble has been reached in current state of the art simulations such as [1, 4, 5]. The rounding errors can be modeled as

\[
\text{rounding error} \approx \frac{\text{rounding error in evaluating nonlinear term}}{\Delta t}.
\]

As noted before, evaluating the nonlinear term leads to second derivatives of the velocity field. The time step \( \Delta t \) appears in the denominator for the same reason that a method of local order
of accuracy $O(\Delta t^{p+1})$ has global order $p$ and not $p+1$. Increasing the Reynolds number means finer meshes which means smaller time steps $\Delta t$ to keep the computation stable. Decreasing the time step amplifies the effect of rounding errors.

By observing the plots in Figure 2.1 and Figure 2.2 carefully, we may evolve the following rule of thumb. The number of digits lost to rounding errors in the numerical evaluation of the first derivative is approximately $2 \log_{10} M$. If spectral integration is used, the number of digits lost is at most $\log_{10} a$. This latter rule is reasonable because spectral integration relies on the smoothing effect of the solution operator and the width of the Green’s function is approximately $a$. These estimates of loss of precision must be doubled for the second derivative. For the simulation of Section 5, $a \approx 2 \times 10^4$ and $M \approx 10^3$. Therefore the number of additional digits of accuracy obtained using spectral integration is 2 if only first derivatives are taken into account and 4 if second derivatives are also taken into account. The plots in Figure 2.2 show that this estimate may in fact be pessimistic.

The upshot of this discussion is that spectral integration, properly deployed, can protect about 5 digits from rounding errors in turbulence simulations. While that is not a panacea—there can be no panacea for differentiation errors in this difficult problem—it appears sufficient to lift the range of achievable Reynolds numbers by an order of magnitude.

3 The Kleiser-Schumann algorithm

Here we use the boundary value solver of Section 2 to derive a version of the Kleiser-Schumann algorithm [8], which does not use numerical differentiation.

In the Fourier decomposition of the velocity field (1.1), denote the Fourier mode $\hat{u}_{l,n}$ by $(u, v, w)$, after dropping the subscripts $l, n$. The Fourier mode at the end of time step $q$ is denoted by $(u^q, v^q, w^q)$. Similarly, if $H = \omega \times u$ is the nonlinear term, denote its $l, n$-th Fourier mode by $(H_1, H_2, H_3)$. Similarly, $p$ denotes the $l, n$-th Fourier mode of pressure (more precisely,
pressure plus $|u|^2/2$ and $p^q$ denotes that Fourier mode at the end of time step $q$.

The Navier-Stokes equation for the $l,n$-th mode takes the following form:

$$
\frac{\partial u}{\partial t} + H_1 = - \frac{il}{\Lambda_x} p + \frac{1}{Re} \left( D^2 - \alpha^2 \right) u
$$

$$
\frac{\partial v}{\partial t} + H_2 = - \frac{\partial p}{\partial y} + \frac{1}{Re} \left( D^2 - \alpha^2 \right) v
$$

$$
\frac{\partial w}{\partial t} + H_3 = - \frac{in}{\Lambda_z} p + \frac{1}{Re} \left( D^2 - \alpha^2 \right) w
$$

where $\alpha^2 = l^2/\Lambda_x^2 + n^2/\Lambda_z^2$. The incompressibility condition is $(il/\Lambda_x)u + \partial v/\partial y + (in/\Lambda_z)w = 0$. Using the incompressibility condition, we get

$$
\left( D^2 - \alpha^2 \right) p = - \frac{il}{\Lambda_x} H_1 - \frac{\partial H_2}{\partial y} - \frac{in}{\Lambda_z} H_3.
$$

Each of these equations is of the form $dX/dt = f(X) + \Delta X/Re$, with $\Delta = (D^2 - \alpha^2)$. The time discretizations we consider are of the following form [21]:

$$
\frac{1}{\Delta t} \left( \gamma X^{q+1} + \sum_{j=0}^{s-1} a_j X^{q-j} \right) = \sum_{j=0}^{s-1} b_j f(X^{q-j}) + \frac{1}{Re} \Delta X^{q+1}.
$$

(3.1)

The method applies to other discretizations such as Runge-Kutta with little change. Low storage Runge-Kutta schemes, which use only slightly more memory than the Euler method, are more commonly used. The low-storage scheme in [16] uses three sub-steps, is 2nd order in viscous terms and 3rd order in convection terms. The theoretical CFL limit is $\sqrt{3}$ [16] or $\sqrt{3}/3 \approx 0.58$ per sub-step. In comparison, the 3rd order 3 step scheme of the form above has 0.63 as its theoretical CFL limit. There appears to be room for a little progress here, which is why we are opting for multistep methods.

If the equations for the $l,n$-th mode are time-discretized, we get

$$
\left( D^2 - \beta^2 \right) u = Re \left( \bar{H}_1 + U \right) + \frac{il}{\Lambda_x} . p . Re
$$

$$
\left( D^2 - \beta^2 \right) v = Re \left( \bar{H}_2 + V \right) + \frac{\partial p}{\partial y} . Re
$$

$$
\left( D^2 - \beta^2 \right) w = Re \left( \bar{H}_3 + W \right) + \frac{in}{\Lambda_z} . p . Re,
$$

(3.2)

where $\beta^2 = \alpha^2 + \gamma Re/\Delta t$. Here $(u,v,w)$ is the $l,n$-th mode of the velocity field (compare (1.1)) at the end of time step $q + 1$ and likewise with $p$. Here $\bar{H}_i = \sum_{j=0}^{s-1} b_j H_i^{q-j}$ for $i = 1, 2, 3$ and $U = \frac{1}{2\Lambda_x} \sum_{j=0}^{s-1} a_j u^{q-j}$. The coefficients $a_j$ and $b_j$ are from the time discretization (3.1).

The quantities $V$ and $W$ are defined in the same manner as $U$. The pressure Poisson equation takes the form

$$
\left( D^2 - \alpha^2 \right) p = - \frac{il}{\Lambda_x} \bar{H}_1 - \frac{\partial \bar{H}_2}{\partial y} - \frac{in}{\Lambda_z} \bar{H}_3.
$$

(3.3)

We will show how to solve (3.3) and (3.2) without numerical differentiation in the $y$ direction. The quantities

$$
u, v, w, H_1, H_2, H_3$$
are assumed to be available at the end of time steps \( q, q-1, \ldots, q-s+1 \). They are used to compute \( \tilde{H}_i \) and \( U,V,W \). The first step, described at greater length below, is to solve for \( u, du/dy, v, dv/dy, w, dw/dy \) at the end of time step \( q+1 \) using (3.3) and (3.2). Once these quantities are available the vorticity component \( \hat{\omega}_{l,n} \) may be formed using arithmetic operations and \( \mathbf{H} = \omega \times \mathbf{u} \) is available for the next time step.

The equations (3.3) and (3.2) are solved for \( u, du/dy, v, dv/dy, w, dw/dy \) as follows.

- Find a particular solution \( p^* \) of the pressure Poisson equation (3.3) using the boundary value solver of Section 2. Note that \( g = -\tilde{H}_2 \) when that solver is applied and \( \tilde{H}_2 \) is not differentiated numerically.

- Find two solutions \( p_1 \) and \( p_2 \) of the homogeneous part of (3.3), which is \((D^2 - \alpha^2) p = 0\) as described in Section 2. These two solutions can be precomputed and reused at every time step.

- Assume \( p = p^* + c_1 p_1 + c_2 p_2 \) and solve the \( v \) equation of (3.2) with the boundary conditions \( v(\pm 1) = 0 \) using the boundary value solver of Section 2. Since \( c_1 \) and \( c_2 \) are undetermined constants, we may take the solution to be \( v = v^* + c_1 v_1 + c_2 v_2 \), where all of \( v^*, v_1, v_2 \) are zero at the walls. Note that \( p^*, p_1, p_2 \) are not differentiated numerically because the boundary value solver which produces those quantities also produces their derivatives. Alternatively, numerical differentiation can be avoided by using \( p^*, p_1, p_2 \) multiplied by \( Re \) in place of \( g \) in the boundary value solver of Section 2.1. As long as the time step \( \Delta t \) does not change, we may precompute and reuse \( v_1 \) and \( v_2 \). The indeterminate quantities \( c_1 \) and \( c_2 \) are calculated using the zero divergence condition \((il/\Lambda_x)u + \partial v/\partial y + (in/\Lambda_z)w = 0\). More specifically, we must have \( dv/dy = 0 \) at \( y = \pm 1 \) since the no-slip boundary requires \( u = v = w = 0 \) at the walls for all but the mean mode. Note that \( v^*, v_1, v_2 \) are not differentiated numerically to enforce \( dv/dy = 0 \) at the walls. The boundary value solver that produces those quantities also produces their derivatives.

- Once we have \( p \), we may solve the \( u \) and \( w \) equations of (3.2) to produce \( u, du/dy \) as well as \( w, dw/dy \).

To complete the description of this method, we show how the mean modes are handled. The mean Fourier components are denoted using an over-bar. The equations for the mean modes at the end of time step \( q+1 \) are as follows:

\[
\left( D^2 - \frac{\gamma Re}{\Delta t} \right) \bar{u} = Re \left( P + \tilde{H}_1 + U \right)
\]

\[
\frac{d\bar{p}}{dy} = -\bar{H}_2
\]

\[
\left( D^2 - \frac{\gamma Re}{\Delta t} \right) \bar{w} = Re \left( \tilde{H}_3 + W \right)
\]

Here \( \tilde{H}_i = \sum_{j=0}^{s-1} b_j \tilde{H}_i^{q-j} \), \( U = \frac{1}{\Delta y} \sum_{j=0}^{s-1} a_j \bar{u}^{q-j} \), and likewise for \( W \). The contribution of the pressure gradient is \( P \), which is set to zero for plane Couette flow. For channel flow the pressure gradient may be fixed at \(-2/Re \), but turbulence is better sustained by fixing the mass flux.
\[ \frac{1}{2} J_{y=\pm 1} \bar{u} dy \text{ at } 2/3 \]. The mass flux is maintained by choosing
\[ p_y = -\frac{1}{2} \int_{-1}^{+1} \tilde{H}_1 dy + \frac{1}{2Re} \frac{\partial \bar{u}}{\partial y} \bigg|_{y=\pm 1} . \]

In either case the laminar solution is \( \bar{u} = (0, 1 - y^2, 0) \). In the equations above, \( P = \sum_{j=0}^{s-1} b_j p_y^{g,j} \). The boundary condition for \( \bar{u} \) is \( \bar{u}(\pm 1) = 0 \) for channel flow and \( \bar{u}(\pm 1) = \pm 1 \) for plane Couette flow. These three equations for the mean mode are uncoupled. The second equation is solved for \( \bar{p} \). From the other two equations, \( \bar{u}, \bar{w} \) as well as their derivatives are obtained using the boundary value solver of Section 2.1. The mean component \( \bar{v} \) is zero as a consequence of incompressibility of the fluid and the no-slip boundary.

4 The Kim-Moin-Moser algorithm

In its classical version, the Kim-Moin-Moser method is slightly more efficient than Kleiser-Schumann in updating the velocity field, although much of the computing time is spent in evaluating the nonlinearity or in moving data between nodes and these are the same for the two methods. There is not much to choose between the two methods in their spectral integration versions. Kim-Moin-Moser relies more on simplifications that are specific to rectangular geometries than Kleiser-Schumann. Generalizations of the Green’s function technique to pipes, boundary layers, and other geometries are more feasible through the Kleiser-Schumann route. In addition, the spectral integration version of Kleiser-Schumann has a more regular form. Therefore the method we have implemented is Kleiser-Schumann. The development of the spectral integration version of Kim-Moin-Moser given in this section will be briefer, but missing details can be filled in by consulting [20].

To begin with, we assume that the wall-normal velocity \( v(x, y, z) \) as well as its derivatives \( \partial v/\partial y \) and \( \partial^2 v/\partial y^2 \), the wall-normal vorticity \( \omega_y(x, y, z) \), its derivative \( \partial \omega_y/\partial y \), and \( H \) are available at the end of time steps \( q, \ldots, q-s+1 \). These quantities are recalculated—without numerical differentiation in the \( y \) direction—at the end of time step \( q+1 \).

As explained in [21], the time discretized Kim-Moin-Moser equations for the mean components are as follows:

\[
\left( D^2 - \gamma Re \frac{\Delta t}{\Delta t} \right) \bar{u} = Re \left( -P + \tilde{H}_1 + U \right) \\
\left( D^2 - \gamma Re \frac{\Delta t}{\Delta t} \right) \bar{w} = Re \left( \tilde{H}_3 + W \right)
\]

The boundary value solver of Section 2.1 is applied to calculate \( \bar{u}, \bar{d}\bar{u}/dy \) and \( \bar{w}, \bar{d}\bar{w}/dy \). The quantities \( P, \tilde{H}_1, U, \) and \( W \) are defined as before.

Let us denote the \( l, n \)-th Fourier component of \( \mathbf{u} \) by \( (u, v, w) \) and \( l, n \)-th Fourier component of \( \nabla \times \mathbf{u} \) by \( (\omega_x, \omega_y, \omega_z) \) (compare (1.1)). The time discretized Kim-Moin-Moser equations for the \( l, n \)-th Fourier mode at the end of time step \( q+1 \) are (compare [21]) as follows:

\[
\left( D^2 - \beta^2 \right) \omega_y = Re \left( \tilde{H}_4 + \Omega_y \right) \tag{4.1}
\]
\[
\left( D^2 - \alpha^2 \right) \left( D^2 - \beta^2 \right) v = Re \left( \tilde{H}_5 + \left( D^2 - \alpha^2 \right) V \right). \tag{4.2}
\]
Here $V$ is as before, but $\tilde{H}_4$, $\tilde{H}_5$, and $\tilde{\Omega}_y$ need to be defined. Let $(H_1, H_2, H_3)$ denote the $l, n$-th Fourier mode of $H$ as before. Then $H_4$ and $H_5$ are defined by

$$H_4 = \frac{in}{\Lambda_z} H_1 - \frac{il}{\Lambda_x} H_3 \quad \text{and} \quad H_5 = -\alpha^2 H_2 - \frac{il}{\Lambda_x} \frac{\partial H_1}{\partial y} - \frac{in}{\Lambda_z} \frac{\partial H_3}{\partial y},$$

respectively. If superscripts stand for time steps as before, $\tilde{H}_i = \sum_{j=0}^{s-1} b_j H_i^{q-j}$ for $i = 4, 5$. Similarly, $\tilde{\Omega}_y = \sum_{j=0}^{s-1} b_j \omega_0^{q-j}$. Here the coefficients $b_j$ are from the time discretization (3.1).

The wall-normal vorticity equation (4.1) is solved in the form

$$D\omega_y - \beta^2 \int \omega_y = \int Re \left( \tilde{H}_4 + \tilde{\Omega}_y \right)$$

by expanding $D\omega_y$ in a Chebyshev series. A particular solution is found using the integral conditions $\mathcal{T}_0 (\omega_y) = \mathcal{T}_0 (D\omega_y) = 0$. Two homogeneous solutions are found satisfying $\mathcal{T}_0 (\omega_y), \mathcal{T}_0 (D\omega_y) = 1, 0$ and $\mathcal{T}_0 (\omega_y), \mathcal{T}_0 (D\omega_y) = 0, 1$, respectively. The homogeneous solutions are linearly combined with the particular solution to enforce the boundary conditions $\omega_y(\pm 1) = 0$ (see [20]).

The wall-normal velocity equation (4.2) is solved in the form

$$\tilde{v} - \beta^2 \int \int \tilde{v} = \int \int Re \left( \tilde{H}_5 + \left( D^2 - \alpha^2 \right) V \right)$$

$$D^2 v - \alpha^2 v = \tilde{v}.$$ 

The first of these equations is solved by expanding $\tilde{v}$ in a Chebyshev series. Notice that the form of this first equation eliminates $y$ derivatives on the right hand side. The second equation is solved by expanding $D^2 v$ in a Chebyshev series.

A particular solution for $\tilde{v}$ is found using the integral conditions $\mathcal{T}_0(\tilde{v}) = \mathcal{T}_1(\tilde{v}) = 0$. This $\tilde{v}$ is used in the right hand side of the second equation to find a particular solution for $v$ with the boundary conditions $\mathcal{T}_0(v) = \mathcal{T}_0(Dv) = 0$. Notice that the integrals on the right hand side of the first equation eliminate $y$ derivatives.

The first two homogeneous solution for $v$ are found by solving $(D^2 - \alpha^2) v = 0$ with the integral conditions $\mathcal{T}_0(v), \mathcal{T}_1(Dv) = 1, 0$ and $\mathcal{T}_0(v), \mathcal{T}_1(Dv) = 0, 1$, respectively. To find two more homogeneous solutions, we solve $\tilde{v} - \beta^2 \int \tilde{v} = 0$ subject to the integral conditions $\mathcal{T}_0(\tilde{v}), \mathcal{T}_1(\tilde{v}) = 1, 0$ and $\mathcal{T}_0(\tilde{v}), \mathcal{T}_1(\tilde{v}) = 0, 1$, respectively. The corresponding $v$ are found by solving $(D^2 - \alpha^2) v = \tilde{v}$ with the boundary conditions $v(\pm 1) = 0$.

The solution of (4.2) for the wall-normal velocity $v$ is found by linearly combining the particular solution with the four homogeneous solutions to satisfy the boundary conditions $v(\pm 1) = dv/dy(\pm 1) = 1$. These four conditions determine the coefficients of the four homogeneous solutions. As explained at length in [20], this peculiar way of computing the homogeneous solutions leads to dramatic cancellation in discretization errors. The key point is that the homogeneous solutions and the particular solution are computed using the same tridiagonal systems. If the homogeneous solutions are computed using an exact formula, for example, the solutions will be accurate only if the grid is fine enough to resolve the numerical boundary layer width of $\beta^{-1}$, and the method will not work well if used to integrate turbulent channel flow or plane Couette flow.

If $(u, v, w)$ are the $l, n$-th Fourier components of $u$ and $(\omega_x, \omega_y, \omega_z)$ of $\nabla \times u$, then at the end of $q + 1$st time step, we can solve the Kim-Moin-Moser equations to compute $v, dv/dy, d^2v/dy^2$.
and $\omega_y, \frac{d\omega_y}{dy}$ without numerical differentiation, as just described, for each $l, n$. We may use the zero divergence condition $(il/\Lambda_y)u + \frac{dv}{dy} + (in/\Lambda_z)w = 0$ along with $\omega_y = \frac{in}{\Lambda_x}u - \frac{il}{\Lambda_y}w$ to solve for $u$ and $w$. In addition, we can compute the derivatives $\frac{du}{dy}$ and $\frac{dv}{dy}$ without numerical differentiation using $\frac{d\omega_y}{dy}$ and $\frac{d^2v}{dy^2}$. From that point, the vorticity $\nabla \times \mathbf{u}$ and the nonlinear term $\mathbf{H}$ can be computed using arithmetic operations.

5 Numerical results

The Reynolds number $Re$ in the Navier-Stokes equation $\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{\Delta \mathbf{u}}{Re}$ is given by $Uh/\nu$ where $U$ is the laminar centerline velocity and $h$ is the channel half width. For wall bounded turbulent flows, the frictional Reynolds number $Re_\tau$ is of greater use. Like the frictional speed $u_\tau$, it is based on the mean shear at the wall. Quantities in frictional units are denoted using $+$ as a superscript. The eddy turnover time $\tau_{eddy}$ is $h/u_\tau$. It is a useful metric for gauging adequacy of the length of integration of the turbulent state [4][5]. A run for gathering statistics should last for $8\tau_{eddy}$ or longer.

Many turbulence phenomena, such as the logarithmic law of the wall, manifest themselves even at low Reynolds numbers such as $Re_\tau = 180$ [7]. It is becoming increasingly clear that large structures and other phenomena emerge as $Re_\tau$ increases. Many engineering applications are in the large $Re_\tau$ regime.

A few of the large $Re_\tau$ simulations are summarized by del Álamo and others [2]. That article reaches $Re_\tau = 1900$ using an $M = 768$ Chebyshev grid in the wall-normal $y$ direction. Hoyas and Jiménez [4][5] reached $Re_\tau = 2003$ using $M = 632$. A higher $Re_\tau$ is reached with fewer grid points because the Hoyas-Jiménez wall-normal grid has 1.5-th power clustering instead of quadratic clustering at the endpoints $y = \pm 1$.

We demonstrate the spectral integration version of Kleiser-Schumann derived in Section 3 in a simulation with $Re_\tau = 2380$ and $M = 1024$. To the best of this author’s knowledge, the Chebyshev grid with $M = 1024$ used in the demonstration is as fine as any wall-normal grid used in earlier turbulence simulations. The algorithm can certainly go beyond $M = 1024$. In fact, the discussion in Section 2 suggests that even $M = 1024 \times 10$, with $a$ or $\beta$ being $10^5$ or so, can be handled effectively. However, this being a 3D computation, problem sizes can rapidly go out of reach of even supercomputers.

The computations described in this section were run on 10 compute nodes, each a 2.67 GHZ Xeon 5650 with 12 processor cores, connected over QDR Infiniband network. The peak memory bandwidth (for reading data) on a single node is more than 30 GB/s. The peak bidirectional network bandwidth on a single node approaches 5 GB/s. Each node has 48 GB of memory. The largest computation carried out used $10^9$ grid points to reach $Re_\tau = 2380$.

A computation of that size uses 35 GB of memory on each node and takes approximately 16 seconds per time step. The time steps are adapted to keep the CFL number in the range $[0.23, 0.27]$. Changes to time step are infrequent and do not incur a significant overhead. Of the 16 seconds taken by a single time step, approximately 3 seconds are for the Kleiser-Schumann step, the topic of this paper, 3 seconds for FFT, and 7 seconds for networking. The rest of the time is taken by accumulating averages (which takes 0.7 seconds per step even though averages are accumulated only once every 100 steps) and arithmetic involved in computing the nonlinear terms and in time stepping. Of all these items, networking is the only one amenable to significant further optimization. Available hardware is quite fully utilized. Larger
5 Numerical results

| $Re$ | $Re_\tau$ | $\Lambda_x$ | $\Lambda_z$ | $L/M/N$ | $dx^+/dy_{max}^+/dz^+$ | $T_{init}u_\tau/h$ | $Tu_\tau/h$ | CFL |
|------|-----------|-------------|-------------|--------|----------------------|------------------|-------------|-----|
| 16875 | 601       | 2           | 1           | 384/320/384 | 9.8/5.9/4.9         | $\geq 30$       | 40.86       | 0.25 |

Tab. 1: Run parameters for validation. Grid spacings in frictional units are $dx^+/dy_{max}^+/dz^+$. The time of integration for eliminating transients is $T_{init}$ and the time of integration for gathering statistics is $T$. CFL is the typical Courant-Friedrichs-Lewy number of a time step.

Computations using more hardware will be given after further algorithmic developments. Xeon Phi/GPU accelerators available today are limited by PCI bus bandwidth. In this memory intensive problem, their utility is limited to the Kleiser-Schumann step.

### 5.1 Validation

The spectral integration method and its implementation were tested in a number of ways. Each module was checked for accuracy and correctness. All the periodic and relative periodic orbits of transitional Couette flow reported in [19] were reproduced with reported accuracy. Moser, Kim, and Mansour (MKM) [10] carried out direct numerical simulations of channel flow at $Re_\tau = 587$. The simulation was state of the art at its time and was reported with considerable care. We use it as the primary basis for validation.

The run parameters of Table 1 are the same as that of MKM with minor differences. The Reynolds number $Re_\tau = 601$ is slightly higher and the grid in the wall-normal direction is finer using $M = 320$ instead of $M = 256$. For second order statistics, the grid resolutions are required to be $dx^+ \approx 9$, $dy_{max}^+ \approx 7$, and $dz^+ \approx 5^2$. The initial run to eliminate transients and achieve a statistically steady turbulent state satisfies $T_{init} \geq 30 \tau_{eddy}$. Thirty eddy turnover times is quite a long integration and we may be sure that transients are thoroughly eliminated.

Figure 5.1 shows excellent agreement of mean streamwise velocity, turbulence intensities, and vorticity fluctuations. The slight discrepancy in streamwise turbulence intensity $u'_{max}$ visible near $y/h \approx 0.4$ is most likely because the MKM run was not as long as that of Table 1. A run with $T > 40 \tau_{eddy}$ is affordable on even a small cluster purchased in 2010, thanks to 15+ years of exponential increase in computing power, but would not have been affordable to MKM. The slight discrepancy in streamwise turbulence intensity near $y/h \approx 1$ is probably because the $Re_\tau$ in Table 1 is slightly higher than that of MKM.

The correlations shown in Figure 5.2 are another validation check. The correlations converge quite slowly, with errors inversely proportional to the time of integration or worse. Here too the agreement is quite good. In general, MKM data seems to have slightly stronger nearby correlations compared to that of Table 1. This suggests that the MKM correlations were smoothened out during the longer time of integration we employed.

### 5.2 Eliminating transients

At large $Re_\tau$, producing a statistically steady initial turbulent state can be as challenging as time stepping the turbulent state. The Kim-Moin-Moser simulation [7] began with an initial field generated using large eddy simulation. In contrast, the most obvious method for

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2 Thanks to a referee of part I of this sequence for this valuable information.
Fig. 5.1: Validation of run of Table 1 against data from [10], which is dotted. The plots show mean streamwise velocity, rms turbulence intensities, and rms vorticity fluctuations as a function of the distance from the wall.

Fig. 5.2: Further validation of run of Table 1 against data from [10], which is dotted/thicker.
generating an initial field is to start with the laminar state, add a little perturbation to it, and integrate long enough. Simple as this may sound, this method was not feasible for state of the art simulations at the time of Kim et al. and it is not feasible today.

The difficulties in reaching a fully developed turbulent state beginning with laminar + perturbation initial state were already encountered by Orszag and Kells [13] in 1980 and may be better appreciated in light of later research. Orszag and Kells found that the laminar + perturbation initial state evolved slowly for a little while and then developed very abrupt transitional instabilities. van Veen and Kawahara [18] have computed homoclinic orbits in transitional Couette flow. It appears that the flow may pass through such homoclinic orbits before it reaches a statistically steady turbulent state. These homoclinic orbits have much finer scales than steady turbulence and are hard to resolve even at the low Reynolds numbers employed by van Veen and Kawahara.

Further insight into transitional instabilities has been provided by Waleffe and others [22, 23]. Fully developed turbulence is characterized by a wide range of scales, coherent structures, spatially intermittent vorticity, and rapid fluctuations that are totally unlike laminar flow. Therefore it is unreasonable to expect analysis of the laminar flow to explain anything but the very beginning of transition. The laminar flow appears to be separated from statistically steady turbulence by a highly complex sequence of instabilities. Waleffe [22] has hypothesized that certain exact coherent structures may be related to some of these instabilities. Critical layers that these exact coherent structures develop as $Re \to \infty$ [23] may be of particular interest. The instabilities that make it very difficult to transition from a laminar + perturbation initial state to statistical turbulence at high $Re$ seem to be strongly localized in space in a manner reminiscent of the critical layer. In this context, it may be mentioned that Sreenivasan [17] has argued for the relevance of transitional critical layers to fully developed turbulent boundary layers.

If large eddy simulation is not an option, two methods may be employed to generate initial states within a turbulent ensemble. One is to compute a fully turbulent state at low $Re$ and then increase $Re$ gradually. The other is to obtain an under-resolved turbulent state and then increase the resolution gradually. The two methods may be used in combination.

The initial states for the two runs of Table 2 were obtained by combining the two methods. The purpose of the runs is to assess how short a $T_{init}$ for eliminating transients suffices at the highest Reynolds number and the finest mesh. In those two runs, it takes approximately $10^5$ time steps to integrate for a single eddy turnover time $\tau_{eddy}$ and each step takes 16 seconds. Thus a reduction in $T_{init}$ is of much value.

Both runs began with an initial state that was generated at the coarser $512^3$ resolution. In the first run, $T_{init} = 0.1\tau_{eddy}$ and in the second run $T_{init} = 2.88\tau_{eddy}$. The times $T$ used to gather statistics were $2.78\tau_{eddy}$ and $2.06\tau_{eddy}$, respectively. Typically, $T \geq 8\tau_{eddy}$ is needed for reliable statistics [4, 5], but here we settle for smaller $T$ to better assess the effect of $T_{init}$.

| $Re$  | $Re_x$ | $\Lambda_x$ | $\Lambda_z$ | $L/M/N$ | $dx^+/dy_{max}^+/dz^+$ | $T_{init}u_x/h$ | $Tu_x/h$ | CFL |
|------|--------|-------------|-------------|---------|---------------------|----------------|----------|-----|
| 80,000 | 2391   | $4/2\pi$   | $2/2\pi$   | 1024/1024/1024 | 9.3/7.3/4.7       | 0.1            | 2.78     | 0.25 |
| 80,000 | 2385   | $4/2\pi$   | $2/2\pi$   | 1024/1024/1024 | 9.3/7.3/4.6       | 2.88           | 2.06     | 0.25 |

Tab. 2: Run parameters for two runs to test elimination of transients. The columns have the same meaning as in Table 1.
Fig. 5.3: Comparison of the two runs of Table 2. A longer run is used to eliminate transients in the second run and plots corresponding to it are thicker.

The first two plots of Figure 5.3 show that larger $T_{\text{init}}$ in the second run does not lead to statistics of better quality. In fact, the turbulence intensities, especially $u'^+$, are better converged for the first run most probably because it is gathering statistics using a larger $T$.

The third plot of the same figure compares the shear at the wall as a function of time for the two runs. In the first run, the magnitude of the shear is greater than 75 but begins to decay right away. That is a telltale sign of the coarser grid origin of the initial state. Coarser grid simulations are more turbulent and have greater shear because there is less viscosity to smooth the flow in a coarser simulation. But already at $t \approx 0.5\tau_{\text{eddy}}$ the first run seems to have reached a statistically steady turbulent state (or more precisely, a sample from a statistically steady turbulent ensemble). It appears that $T_{\text{init}} \in [0.5\tau_{\text{eddy}}, 1.0\tau_{\text{eddy}}]$ suffices to eliminate transients from an initial state computed at lower resolution.

A simulation with $T \geq 8\tau_{\text{eddy}}$, adequate for reliable second order statistics, will take four more months of computing and will be included at a later time.

6 Conclusion

The work of Kim, Moin, and Moser [7] (1987) showed that fully turbulent solutions of the Navier-Stokes equation with walls as boundaries are amenable to computation. A salient feature of this line of work is the detailed agreement between computations and experiment. Since then, simulations have used finer and finer grids to reach higher Reynolds numbers.

As computational grids are refined, discretization errors decrease and rounding errors increase. When the point where rounding errors overtake discretization errors is reached, refining
the grid becomes futile, indeed harmful, and higher Reynolds numbers cannot be reached.

The point where rounding errors dominate has been reached in simulations of turbulent channel flow and more generally wall bounded turbulence. In this paper, the classical Kleiser-Schumann and Kim-Moin-Moser methods are re-derived to ameliorate the rounding errors that arise from differentiation in the wall-normal direction. In both these methods, the dominant contribution to rounding error comes from wall-normal differentiation. The spectral integration version of Kleiser-Schumann method has been derived, implemented, and applied to turbulent channel flow using $10^9$ grid points in total and $1024$ in the wall-normal direction. The Reynolds numbers reached is $Re_\tau = 2380$. The method appears capable of reaching Reynolds numbers that are an order of magnitude higher.

The hardware used in the present paper consisted mainly of 10 compute nodes of a small cluster purchased in 2010. Single compute nodes capable of handling $10^9$ grid points in turbulence simulations are already available and will become increasingly common. In computations of that scale and beyond, the rounding errors begin to dominate and the algorithms derived here will be found useful.

In part III of this sequence, another method for reaching higher Reynolds numbers will be presented. That method will use Green’s functions explicitly as in part I [21] with a Hoyas-Jiménez type wall-normal grid. Simulations at larger $Re_\tau$ will be given in that article.

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