A Pseudo-Spectral Method for Numerical Simulation of Incompressible Flows

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Abstract

A pseudo-spectral method, developed by Dumas & Leonard(1), to study incompressible flows of viscous fluids is reported. The unique feature of this method is the altogether elimination of pressure from the Navier-Stokes equation. The example spherical Couette flow is chosen for the purpose of demonstration.

INTRODUCTION

An ongoing investigation of vortices in spherical annulus has motivated the compilation of this report. Since several simple incompressible flows are usually described by the velocity and pressure fields, solving the Navier-Stokes equation is inescapable. Although, quite often one is interested only in the velocity field. This report is concerned with a pseudo-spectral method to eliminate pressure from the Navier-Stokes equation altogether.

Spectral methods are spatial discretization methods wherein the sought function is approximated by a linear combination of ansatz functions with unknown coefficients. These coefficients are sought as solution such that the error generated due to the approximation is minimized. The distinguishing feature of spectral methods is the global support of ansatz functions, due to which spectral approximations converge exponentially.

The presented method is "pseudo"-spectral due to the non-linear term which requires few computations to be performed in physical space. From a programming perspective, the transformations between physical and spectral space are crucial to the speed. Fortunately, several libraries exist (written in FORTRAN/C), that perform this task efficiently.

This report is broadly divided in two sections. The first section presents the method with some necessary background, while the second one demonstrates the application of this method to spherical Couette flow. This example is instrumental in understanding flows in spherical geometry and also for the purpose of validation.

THEORY

An incompressible flow of viscous fluid is mathematically modeled by the Navier-Stokes and continuity equation. In a dimensionless form, they are

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \frac{1}{Re} \nabla^2 \boldsymbol{u} \tag{1}$$

$$\nabla \cdot \boldsymbol{u} = 0 \tag{2}$$

where $\boldsymbol{u}(\boldsymbol{r}, t)$ is the velocity field, $p(\boldsymbol{r}, t)$ is the pressure field and Re is the Reynold's number. It would later help to express the non-linear term as

$$\boldsymbol{u} \cdot \nabla \boldsymbol{u} = \frac{1}{2} \nabla (\boldsymbol{u} \cdot \boldsymbol{u}) - \boldsymbol{u} \times (\nabla \times \boldsymbol{u}). \tag{3}$$

Therefore, equation (1) can be written as

$$\frac{\partial \boldsymbol{u}}{\partial t} = -\nabla P + \frac{1}{Re} \nabla^2 \boldsymbol{u} + \boldsymbol{F} \tag{4}$$

where, $P = p + (\boldsymbol{u} \cdot \boldsymbol{u}/2)$ and $\boldsymbol{F} = \boldsymbol{u} \times (\nabla \times \boldsymbol{u})$. Since the non-linear term is most often treated explicitly in discrete time-integration, $\boldsymbol{F}$ can be viewed as a *forcing* term.

Before introducing the pressure elimination method, a brief discussion of WRMs is necessary.

WEIGHTED RESIDUAL METHODS

WRMs is a collective name for a class of methods used to solve equations of the form

$$\mathcal{L}(\boldsymbol{u}) - \boldsymbol{f} = 0 \qquad \text{in} \quad V \tag{5}$$

where $\boldsymbol{u}(\boldsymbol{r})$ is the unknown dependent function, $\boldsymbol{f}(\boldsymbol{r})$ is a known vector-function, $\mathcal{L}$ is an operator involving derivatives of $\boldsymbol{u}(\boldsymbol{r})$ and V is the solution domain.

The first step in a WRM is to approximate $\boldsymbol{u}$ with some known function(s) based on its general behavior and the boundary conditions. Next, this approximate solution is substituted in equation (5). Being an approximation, equation (5) is not satisfied exactly over the entire solution domain and consequently, a residue is produced. Thus, if

$$\boldsymbol{u} \approx \bar{\boldsymbol{u}} \tag{6}$$

then

$$\mathcal{L}(\bar{\boldsymbol{u}}) - \boldsymbol{f} = \boldsymbol{R} \qquad \text{in} \quad V \tag{7}$$

where $\boldsymbol{R}$ is the residue and is a measure of the error due to approximation. The goal of any WRM is to make $\boldsymbol{R}$ vanish over the solution domain in an *average* sense. To this end, an inner product is defined in the following manner

$$\langle \boldsymbol{R}, \boldsymbol{\psi} \rangle \equiv \int_V \boldsymbol{R} \cdot \boldsymbol{\psi} \, \mathrm{d}V = 0 \tag{8}$$

where $\boldsymbol{\psi}(\boldsymbol{r})$ is usually known as the test function that determines the *sense of averaging.* The choice of $\boldsymbol{\psi}$ depends on the particular problem at hand.

In spectral methods, $\boldsymbol{u}$ is approximated by a linear combination of a finite set of known *basis* functions,

$$\boldsymbol{u}(\boldsymbol{r}) = \sum_{i=0}^{N} a_i \boldsymbol{u}_i(\boldsymbol{r}) \tag{9}$$

where, the coefficients a_i are sought as the solution. The test function is also expressed as a linear combination of another set,

$$\boldsymbol{\psi}(\boldsymbol{r}) = \sum_{i=0}^{N} w_i \boldsymbol{\psi}_i(\boldsymbol{r}). \tag{10}$$

Traditionally, it is assumed that $\boldsymbol{u}$ and consequently $\boldsymbol{u}_i$ satisfy homogeneous boundary conditions so that any set a_i satisfies (9). However, for a solution that satisfies non-homogeneous boundary conditions, the following decomposition is used.

$$\boldsymbol{u} = \sum_{i=0}^{N} a_i \boldsymbol{u}_i + \boldsymbol{u}_{bc}, \tag{11}$$

where $\boldsymbol{u}_i$ satisfy *homogeneous* boundary condition while $\boldsymbol{u}_{bc}$ is any function that satisfies the actual boundary conditions.

Combining equations (7), (8), (10) and (11), we get

$$\sum_{n=0}^{N} a_n \langle \mathcal{L}(\boldsymbol{u}_n), \boldsymbol{\psi}_i \rangle + \langle \mathcal{L}(\boldsymbol{u}_{bc}), \boldsymbol{\psi}_i \rangle - \langle \boldsymbol{f}, \boldsymbol{\psi}_i \rangle = 0, \tag{12}$$

$0 \leq i \leq N$. One would like the matrix $\mathrm{L}_{in} = \langle \mathcal{L}(\boldsymbol{u}_n), \boldsymbol{\psi}_i \rangle$ to be as "diagonal" as possible. Thus, the choice of basis and test functions becomes crucial.

ELIMINATION OF PRESSURE

In the light of (8), consider the inner product of (4) with $\boldsymbol{\psi}$

$$\langle \frac{\partial \boldsymbol{u}}{\partial t}, \boldsymbol{\psi} \rangle = -\langle \nabla P, \boldsymbol{\psi} \rangle + \frac{1}{Re} \langle \nabla^2 \boldsymbol{u}, \boldsymbol{\psi} \rangle + \langle \boldsymbol{F}, \boldsymbol{\psi} \rangle. \tag{13}$$

Now, with the vector identity

$$\boldsymbol{\psi} \cdot \nabla P = \nabla \cdot (P \boldsymbol{\psi}_j) - P(\nabla \cdot \boldsymbol{\psi}_j) \tag{14}$$

and the Gauss' theorem

$$\int_V (\nabla \cdot \boldsymbol{a}) \, \mathrm{d}V = \int_S (\boldsymbol{a} \cdot \boldsymbol{n}) \, \mathrm{d}S \tag{15}$$

where $\boldsymbol{n}$ is the outward unit normal vector to S (boundary of V), the pressure term can be expressed as

$$\langle \nabla P, \boldsymbol{\psi} \rangle = \int_S P(\boldsymbol{\psi} \cdot \boldsymbol{n}) dS - \int_V P(\nabla \cdot \boldsymbol{\psi}) dV. \tag{16}$$

Therefore, if

$$\nabla \cdot \boldsymbol{\psi} = 0 \tag{17}$$

and

$$\boldsymbol{\psi} \cdot \boldsymbol{n} = 0, \tag{18}$$

that is it satisfies the no-through flow condition, then the term $\langle \nabla P, \boldsymbol{\psi} \rangle$ is identically zero. Thus, the working equation becomes

$$\langle \frac{\partial \boldsymbol{u}}{\partial t}, \boldsymbol{\psi} \rangle - \frac{1}{Re} \langle \nabla^2 \boldsymbol{u}, \boldsymbol{\psi} \rangle = \langle \boldsymbol{F}, \boldsymbol{\psi} \rangle \tag{19}$$

This equation is valid for any incompressible flow of viscous fluid and is derived without any regard to geometry. We proceed further by illustrating the application of this method to problem of spherical Couette flow. This problem shall help to realise the scope of application of this method.

SPHERICAL COUETTE FLOW

In this report, spherical Couette flow is defined as follows:
The incompressible flow of a viscous fluid in between two concentric spheres of radii R_i and R_o undergoing differential rotation with angular velocities $\Omega_i(t)$ and $\Omega_o(t)$ and an angle of $\alpha_o(t)$ between their rotation axes. In spherical polar coordinates (r, θ, ϕ) the boundary conditions for velocity field are written as

$$\begin{aligned} \boldsymbol{u}(r = R_i, \theta, \phi) &= \Omega_i R_i \sin\theta \, \hat{\boldsymbol{e}}_{\boldsymbol{\phi}} \\ \boldsymbol{u}(r = R_o, \theta, \phi) &= \Omega_o R_o [(-\sin\alpha_o \sin\phi) \, \hat{\boldsymbol{e}}_{\boldsymbol{\theta}} \\ &\quad + (\cos\alpha_o \sin\theta - \sin\alpha_o \cos\theta \cos\phi) \, \hat{\boldsymbol{e}}_{\boldsymbol{\phi}}] \end{aligned} \tag{20}$$

Thus, given a $\boldsymbol{\psi}$ that satisfies (17) and (18), we seek a velocity field that satisfies (2) and (19) subject to the boundary conditions (20) and initial conditions

$$\begin{aligned} \Omega_o(0) &= \Omega_o \\ \Omega_i(0) &= \Omega_i \\ \alpha_o(0) &= \alpha_o \end{aligned} \tag{21}$$

where Ω_o, Ω_i and α_o are known.

Before going any further, all the variables are non-dimensionalised by choosing $d = R_o - R_i$ as the reference length and $\Omega_o R_o$ as the reference velocity. Henceforth, all the variables must be viewed as dimensionless.

VECTOR EXPANSION

Velocity and test function are constructed as products of one-dimensional functions of space and time, i.e.,

$$\begin{aligned} \boldsymbol{v}(r, \theta, \phi, t) = \sum_{n=0}^{N} \sum_{l=0}^{L} \sum_{m=0}^{M} \{ & \hat{v}^r_{nlm}(t) \, \mathrm{R}_n(r) \, \Theta_l(\theta) \, \Phi_m(\phi) \, \hat{\boldsymbol{e}}_{\boldsymbol{r}} + \hat{v}^\theta_{nlm}(t) \, \mathrm{R}_n(r) \, \Theta_l(\theta) \, \Phi_m(\phi) \, \hat{\boldsymbol{e}}_{\boldsymbol{\theta}} \\ & + \hat{v}^\phi_{nlm}(t) \, \mathrm{R}_n(r) \, \Theta_l(\theta) \, \Phi_m(\phi) \, \hat{\boldsymbol{e}}_{\boldsymbol{\phi}} \}. \end{aligned} \tag{22}$$

The spatial basis functions are chosen so as to simplify the evaluation of the inner products in (). It should be brought to attention that both, the velocity and the test function, belong to the subspace of divergence-free vector fields. Furthermore, both of them satisfy no-through flow condition at the boundary [see (2),(17),(18) and (20)]. These two facts narrow down the choices.

First, expression of the form (22) for an arbitrary divergence-free vector field is developed. Then the constraint of homogeneous boundary condition is imposed. Based on the expression obtained, velocity and test function are constructed.

ANGULAR DIRECTION

The coordinates θ and ϕ together describe a spherical surface. On such a surface, the family of three orthogonal vector-functions, the vector spherical harmonics, VSHs, can be used to express any arbitrary vector field, i.e.,

$$\boldsymbol{u}(t, r, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \{ H^X_{lm}(r, t) \boldsymbol{X}_{lm}(\theta, \phi) + H^V_{lm}(r, t) \boldsymbol{V}_{lm}(\theta, \phi) + H^W_{lm}(r, t) \boldsymbol{W}_{lm}(\theta, \phi) \} \tag{23}$$

where

$$\boldsymbol{X}_{lm}(\theta, \phi) \equiv \frac{-i}{[l(l+1)]^{1/2}} [\hat{\boldsymbol{e}}_{\boldsymbol{r}} \times (r \nabla Y^m_l(\theta, \phi))] \tag{24}$$

$$\boldsymbol{V}_{lm}(\theta, \phi) \equiv \frac{1}{[(l+1)(2l+1)]^{1/2}} [r \nabla Y^m_l(\theta, \phi) - (l+1) Y^m_l(\theta, \phi) \hat{\boldsymbol{e}}_{\boldsymbol{r}}] \tag{25}$$

$$\boldsymbol{W}_{lm}(\theta, \phi) \equiv \frac{1}{[l(2l+1)]^{1/2}} [r \nabla Y^m_l(\theta, \phi) + l Y^m_l(\theta, \phi) \hat{\boldsymbol{e}}_{\boldsymbol{r}}] \tag{26}$$

are the VSHs constructed with the well-known spherical harmonics $Y_l^m(\theta,\phi)$. They obey the following orthogonality property

$$\int_0^{2\pi}\int_0^{\pi} \boldsymbol{C}_{lm} \cdot \boldsymbol{D^*}_{l'm'} \, \sin\theta \, d\theta \, d\phi = \delta_{\boldsymbol{CD}} \, \delta_{ll'} \, \delta_{mm'} \tag{27}$$

Here, "$*$" denotes the complex conjugate and $\boldsymbol{C}, \boldsymbol{D} \in \{\boldsymbol{X}, \boldsymbol{V}, \boldsymbol{W}\}$. The functions $H_{lm}^X(r,t), H_{lm}^V(r,t)$ and $H_{lm}^W(r,t)$ are still arbitrary. Now, with the following expressions for divergence and curl of VSHs,

$$\begin{aligned}
\nabla \cdot [R(r)\boldsymbol{X}_{lm}] &= 0 \\
\nabla \cdot [R(r)\boldsymbol{V}_{lm}] &= -\left(\frac{l+1}{2l+1}\right)^{1/2} \left[\frac{\mathrm{d}R}{\mathrm{d}r} + \frac{l+2}{r}R\right] Y_l^m \\
\nabla \cdot [R(r)\boldsymbol{W}_{lm}] &= -\left(\frac{l}{2l+1}\right)^{1/2} \left[\frac{\mathrm{d}R}{\mathrm{d}r} - \frac{l-1}{r}R\right] Y_l^m \\
\nabla \times [R(r)\boldsymbol{X}_{lm}] &= i\left(\frac{l}{2l+1}\right)^{1/2} \left[\frac{\mathrm{d}R}{\mathrm{d}r} - \frac{l}{r}R\right] \boldsymbol{V}_{lm} + \\
&\quad i\left(\frac{l+1}{2l+1}\right)^{1/2} \left[\frac{\mathrm{d}R}{\mathrm{d}r} + \frac{l+1}{r}R\right] \boldsymbol{W}_{lm} \\
\nabla \times [R(r)\boldsymbol{V}_{lm}] &= i\left(\frac{l}{2l+1}\right)^{1/2} \left[\frac{\mathrm{d}R}{\mathrm{d}r} + \frac{l+2}{r}R\right] \boldsymbol{X}_{lm} \\
\nabla \times [R(r)\boldsymbol{W}_{lm}] &= i\left(\frac{l+1}{2l+1}\right)^{1/2} \left[\frac{\mathrm{d}R}{\mathrm{d}r} - \frac{l-1}{r}R\right] \boldsymbol{X}_{lm},
\end{aligned}$$

it can be shown that, for a divergence-free field, $H_{lm}^V(r,t)$ and $H_{lm}^W(r,t)$ must be related as

$$H_{lm}^V(r,t) = i\left(\frac{l}{2l+1}\right)^{1/2} \left[\frac{\partial H_{lm}^+(r,t)}{\partial r} - \frac{l}{r}H_{lm}^+(r,t)\right] \tag{28}$$

$$H_{lm}^W(r,t) = i\left(\frac{l+1}{2l+1}\right)^{1/2} \left[\frac{\partial H_{lm}^+(r,t)}{\partial r} + \frac{l+1}{r}H_{lm}^+(r,t)\right] \tag{29}$$

through a common function $H_{lm}^+(r,t)$. Hence, any arbitrary divergence-free vector field can be approximated as

$$\boldsymbol{u}(r,\theta,\phi,t) = \sum_{l=0}^{L}\sum_{m=-1}^{l} \{H_{lm}^-(r,t)\boldsymbol{X}_{lm}(\theta,\phi) + \nabla \times \left[H_{lm}^+(r,t)\boldsymbol{X}_{lm}(\theta,\phi)\right] \tag{30}$$

where the approximation is only due to the truncation.

RADIAL DIRECTION

As mentioned before, the basis functions satisfy homogeneous boundary conditions. This implies that $H_{lm}^\pm(R_i,t)$ and $H_{lm}^\pm(R_o,t)$ must be zero for all pairs (l,m). Keeping this in mind, the radial and time dependence is split as

$$H_{lm}^-(r,t) = \sum_{n=0}^{N} a_{nlm}^-(t) h_n^-(r), \tag{31}$$

$$H_{lm}^+(r,t) = \sum_{n=0}^{N} a_{nlm}^+(t) h_n^+(r) \tag{32}$$

and

$$H_{lm}^V(r,t) = \sum_{n=0}^{N} a_{nlm}^+(t) h_{nl}^{+V}(r), \tag{33}$$

$$H_{lm}^W(r,t) = \sum_{n=0}^{N} a_{nlm}^+(t) h_{nl}^{+W}(r). \tag{34}$$

Further, from (28) and (29), it is not hard to see that

$$h_{nl}^{+V} = i\left(\frac{l}{2l+1}\right)^{1/2}\left[\frac{dh_n^+}{dr} - \frac{l}{r}h_n^+\right] \tag{35}$$

$$h_{nl}^{+W} = i\left(\frac{l+1}{2l+1}\right)^{1/2}\left[\frac{dh_n^+}{dr} + \frac{l+1}{r}h_n^+\right] \tag{36}$$

These functions are required to satisfy the following conditions.

$$h_n^-(R_i) = h_n^-(R_o) = 0, \tag{37}$$

$$h_{nl}^{+V}(R_i) = h_{nl}^{+V}(R_o) = h_{nl}^{+W}(R_i) = h_{nl}^{+W}(R_o) = 0 \tag{38}$$

which implies

$$h_n^+(R_i) = h_n^+(R_o) = \frac{dh_n^+(R_i)}{dr} = \frac{dh_n^+(R_o)}{dr} = 0 \tag{39}$$

Polynomials such as Jacobi, Legendre or Chebyshev are usually orthogonal on the domain [-1,1] and span the space of functions with arbitrary end-point conditions. Chebyshev polynomials, $T_n(\xi)$ $(-1 \leq \xi \leq 1)$, are particularly suitable because their transforms can be implemented with the efficient Fast Fourier transform algorithms. They are orthogonal with respect to the weight function $1/\sqrt{1-\xi^2}$ as

$$\int_{-1}^{1} \frac{1}{\sqrt{1-\xi^2}} T_n(\xi) T_m(\xi) \mathrm{d}\xi = \frac{\pi}{2}\, c_n \delta_{nm} \tag{40}$$

where $c_0 = 2$ and $c_n = 1$ for $n > 0$.

Before proceeding further, it shall be convenient to do the following transformation

$$\xi = 2r - K, \qquad K = R_i + R_o \tag{41}$$

such that

$$[R_i \leq r \leq R_o] \quad \Leftrightarrow \quad [-1 \leq \xi \leq 1]\,.$$

Considering the constraints (37) and (39), the radial basis functions $h_n^-(\xi)$ and $h_n^+(\xi)$ are chosen as

$$h_n^-(\xi) = (1-\xi^2)\, T_n(\xi) \tag{42}$$

$$h_n^+(\xi) = (1-\xi^2)^2\, r T_n(\xi) \tag{43}$$

and from equations (35) and (36), we have

$$h_{nl}^{+V}(\xi) = i\left(\frac{l}{2l+1}\right)^{1/2} \{(1-l)[(1-\xi^2)^2 T_n(\xi)] + (\xi+K)[(1-\xi^2)^2 T_n(\xi)]'\} \tag{44}$$

$$h_{nl}^{+W}(\xi) = i\left(\frac{l+1}{2l+1}\right)^{1/2} \{(2+l)[(1-\xi^2)^2 T_n(\xi)] + (\xi+K)[(1-\xi^2)^2 T_n(\xi)]'\} \tag{45}$$

The factor "r" in h_n^+ is included for analytical convinience. It must be mentioned that the sets h_n^-, h_n^{+V} and h_n^{+W} do not really form a basis since they are not orthogonal. Nevertheless, they do show *quasi-orthogonality*, i.e., the matrix

$$[\mathcal{H}_{nm}]_l = \int_{-1}^{1} h_{nl}(\xi)\, h_{ml}(\xi) \frac{d\xi}{\sqrt{1-\xi^2}}$$

is band-structured because of the fact that both the functions in the integrand (excluding $1/\sqrt{1-\xi^2}$) can be expressed as

$$h_{nl}(\xi) = \sum_{j=-4}^{4} \beta_{lj} T_{n+j}(\xi), \tag{46}$$

where β_{lj} are determined from recurrence relations of Chebyshev polynomials.

Thus, any arbitrary divergence-less field that satisfies homogeneous boundary conditions can be approximated as

$$\boldsymbol{u}(r,\theta,\phi,t)=\sum_{n=0}^{N}\sum_{l=0}^{L}\sum_{m=-l}^{l}\{a^{-}_{nlm}(t)\,h^{-}_{n}(\xi)\,\boldsymbol{X}_{lm}(\theta,\phi)+a^{+}_{nlm}(t)\,h^{+V}_{nl}(\xi)\,\boldsymbol{V}_{lm}(\theta,\phi)$$
$$+\,a^{+}_{nlm}(t)\,h^{+W}_{nl}(\xi)\,\boldsymbol{W}_{lm}(\theta,\phi)\} \tag{47}$$

VELOCITY

To express an arbitrary divergence-free velocity field that satisfies the boundary conditions given in (20), $\boldsymbol{u}_{bc}$ in (11) must be defined. It is not difficult to verify that solid-body rotation at the walls can be expressed in terms of $\boldsymbol{X}_{lm}$ only, with $l=1$. In the radial direction, a simple linear variation (in terms of $T_0(\xi)$ and $T_1(\xi)$) is sufficient. Therefore,

$$\boldsymbol{u}_{bc}(r(\xi),\theta,\phi,t)=\sum_{m=-1}^{1}\left[\Lambda^{0}_{m}(t)T_0(\xi)+\Lambda^{1}_{m}(t)T_1(\xi)\right]\boldsymbol{X}_{1m}(\theta,\phi) \tag{48}$$

where

$$\begin{aligned}
\Lambda^{0}_{0}(t)&=-i\left(\frac{2\pi}{3}\right)^{1/2}\left[\Omega_o(t)R_o\cos(\alpha_o(t))+\Omega_i(t)R_i\right]\\
\Lambda^{1}_{0}(t)&=-i\left(\frac{2\pi}{3}\right)^{1/2}\left[\Omega_o(t)R_o\cos(\alpha_o(t))-\Omega_i(t)R_i\right]\\
\Lambda^{0,1}_{\pm1}(t)&=\pm i\left(\frac{\pi}{3}\right)^{1/2}\Omega_o(t)R_o\sin(\alpha_o(t))
\end{aligned} \tag{49}$$

Finally, combining (47) with (48), the velocity field is approxiamted as

$$\boldsymbol{u}(r,\theta,\phi,t)=\sum_{n=0}^{N}\sum_{l=0}^{L}\sum_{m=-l}^{l}\{a^{-}_{nlm}(t)\,h^{-}_{n}(\xi)\,\boldsymbol{X}_{lm}(\theta,\phi)+a^{+}_{nlm}(t)\,h^{+V}_{n}(\xi)\,\boldsymbol{V}_{lm}(\theta,\phi)+$$
$$a^{+}_{nlm}(t)\,h^{+W}_{n}(\xi)\,\boldsymbol{W}_{lm}(\theta,\phi)\}+\sum_{m=-1}^{1}\left[\Lambda^{0}_{m}(t)T_0(\xi)+\Lambda^{1}_{m}(t)T_1(\xi)\right]\boldsymbol{X}_{1m}(\theta,\phi). \tag{50}$$

TEST FUNCTION

The test function also belongs to the subspace of divergence-free vectors with zero wall-normal component at the boundary. But unlike velocity, it is not required to have any tangential component at the boundary. Therfore, we simply choose a vector-function that satisfies homogeneous boundary condition as our test function, i.e.,

$$\boldsymbol{\psi}(r,\theta,\phi)=\sum_{n'=0}^{N}\sum_{l'=0}^{L}\sum_{m'=-l'}^{l'}\{\,g^{-}_{n'}(\xi)\,\boldsymbol{X^*}_{l'm'}(\theta,\phi)+\,g^{+V}_{n'}(\xi)\,\boldsymbol{V^*}_{l'm'}(\theta,\phi)+g^{+W}_{n'}(\xi)\,\boldsymbol{W^*}_{l'm'}(\theta,\phi)\} \tag{51}$$

where

$$g^{-}_{n'}(\xi)=\frac{1}{\sqrt{1-\xi^2}}\,(1-\xi^2)\,T_{n'}(\xi) \tag{52}$$

$$g^{+}_{n'}(\xi)=\frac{1}{\sqrt{1-\xi^2}}\,(1-\xi^2)^2\,rT_{n'}(\xi) \tag{53}$$

and

$$g^{+V}_{n'l'} = i\left(\frac{l'}{2l'+1}\right)^{1/2}\left[\frac{dg^{+}_{n'}}{dr} - \frac{l'}{r}g^{+}_{n'}\right] \tag{54}$$

$$g^{+W}_{n'l'} = i\left(\frac{l'+1}{2l'+1}\right)^{1/2}\left[\frac{dg^{+}_{n'}}{dr} + \frac{l'+1}{r}g^{+}_{n'}\right] \tag{55}$$

The factor $1/\sqrt{1-\xi^2}$ and the conjugates of VSHs are necessary to utilize orthogonality of Chebyshev polynomials and VSHs in order to simplify the evaluation of inner products in (19).

NON-LINEAR TERM

A general vector expansion in terms of Chebyshev polynomials and VSHs is used to approximate the non-linear term, i.e.,

$$r^2\boldsymbol{F}(r,\theta,\phi) = \sum_{n=0}^{N_d}\sum_{m=-M_d}^{M_d}\sum_{l=|m|}^{L_d}\{f^X_{nlm}T_n(\xi(r))\boldsymbol{X}_{lm}(\theta,\phi) + f^V_{nlm}T_n(\xi(r))\boldsymbol{V}_{lm}(\theta,\phi) + f^W_{nlm}T_n(\xi(r))\boldsymbol{W}_{lm}(\theta,\phi)\}. \tag{56}$$

Here,

$$N_d = \frac{3}{2}(N+4)+1$$
$$L_d = \frac{3}{2}(L+1)+1$$
$$M_d = \frac{3}{2}M+1$$

result from Orszag's 3/2-rule. Inclusion of r^2 in (56) facilitates evaluation of the inner product in (19).

The coefficients f^X_{nlm}, f^V_{nlm} and f^W_{nlm} are obtained from $a^{\pm}_{nlm}$. This process is subject to aliasing (see (2)) wherein non-linear interactions of band-limited spectral information generates frequencies outside the band which cannot be physically interpreted. Therefore, such computations require special treatment.

DE-ALIASING AND STANDARD REPRESENTATION

To illustrate a method of computing the spectral coefficients of non-linear terms, exact atleast upto the cutoff frequency (N), consider two discrete functions

$$U_i = \sum_{n=0}^{N}\hat{u}_nT_n(x_i)$$

and

$$V_i = \sum_{n=0}^{N}\hat{v}_nT_n(x_i)$$

($i = 0, ..., N$) defined on $[-1,1]$, where $T_n(x)$ is the n^{th} order Chebyshev polynomials and $x_i = \cos(i\pi/N)$. One seeks the coefficients,

$$\hat{z}_n = \frac{1}{\gamma_n}\sum_{i=0}^{N}Z_iT_n(x_i)w_i,$$

of the product $Z_i = U_i \cdot V_i$, where $(w_i, \gamma_i) = (\pi/2N, \pi)$ for $n = 0, N$ and $(\pi/N, \pi/2)$ for $0 < i < N$. The procedure of computing alias-free coefficients involves the following steps:

1. The sequences $\hat{u}_n$ and $\hat{v}_n$ ($0 \le n \le N$), are extended upto $N_a = (3/2)N + 1$ (according to Orszag's 3/2-rule) by adding zeros, i.e., $\hat{u}_n = \hat{v}_n = 0$ for $N < n \le N_a$.

2. These coefficients are then forward transformed to obtain U_i and V_i $(0 \leq i \leq N_a)$

3. The product $Z_i = U_i \cdot V_i$ is computed at $N_a + 1$ collocation points and then backward transformed to obtain the $\hat{z}_n (0 \leq n \leq N_a)$, where coefficients upto $n = N$ are guaranteed to be exact.

Step 2 involves computations performed in physical space. Hence, pseudo-spectral method. The transformations between physical and spectral space constitute a major fraction of the total computations and must be performed as efficiently as possible. To this end, routines available in the FORTAN libraries FFTW(3) (for Chebyshev transform) and SHTns(4) (for VSH transform) are used.

Chebyshev transforms require spectral representation in the form

$$\boldsymbol{u}(r, \theta, \phi) = \sum_{n=0}^{N_p} \sum_{l=0}^{L} \sum_{m=-l}^{l} \{u_{nlm}^X T_n(\xi) \boldsymbol{X}_{lm}(\theta, \phi) + u_{nlm}^V T_n(\xi) \boldsymbol{V}_{lm}(\theta, \phi) + u_{nlm}^W T_n(\xi) \boldsymbol{W}_{lm}(\theta, \phi) \tag{57}$$

where $u_{nlm}^X, u_{nlm}^V, u_{nlm}^W$ are obtained from $a_{nlm}^{\pm}$. This conversion entails the following general transformation

$$\sum_{n=0}^{N} a_n h_n(\xi) \Rightarrow \sum_{j=0}^{N_p} u_j T_j(\xi). \tag{58}$$

From equation (46), we can write

$$\sum_{n=0}^{N} a_n h_n(\xi) = \sum_{n=0}^{N} a_n \sum_{i=-4}^{4} \beta_{ni} T_{n+i}(\xi), \tag{59}$$

which upon replacing n with $j = n + i$ becomes

$$\sum_{n=0}^{N} a_n h_n(\xi) = \sum_{j=0}^{N+4} \sum_{i=-4}^{4} a_{(j-i)} \beta_{(j-i)i} T_j(\xi). \tag{60}$$

Thus, on comparing with (58), one can write, for every pair (l, m)

$$\begin{aligned} \{u_{n'}^X\} &= \sum_{n=0}^{N} \left[CU_{n'n}^X\right]_l \{a_n^-\} \\ \{u_{n'}^V\} &= \sum_{n=0}^{N} \left[CU_{n'n}^V\right]_l \{a_n^+\} \\ \{u_{n'}^W\} &= \sum_{n=0}^{N} \left[CU_{n'n}^W\right]_l \{a_n^+\} \end{aligned} \tag{61}$$

$0 \leq n' \leq N + 4$. $[\cdot]$ denotes a two-dimensional array and $\{\cdot\}$ denotes a vector. A similar standard representation for $r(\nabla \times \boldsymbol{u})$ can be obtained in terms of $a_{nlm}^{\pm}$, i.e.,

$$r\nabla \times \boldsymbol{u} = \sum_{n=0}^{N+4} \sum_{l=0}^{L} \sum_{m=-l}^{l} \{s_{nlm}^X T_n(\xi) \boldsymbol{X}_{lm}(\theta, \phi) + s_{nlm}^V T_n(\xi) \boldsymbol{V}_{lm}(\theta, \phi) + s_{nlm}^W T_n(\xi) \boldsymbol{W}_{lm}(\theta, \phi)\}. \tag{62}$$

where, for every pair (l, m)

$$\begin{aligned} \{s_{n'}^X\} &= \sum_{n=0}^{N} \left[CS_{n'n}^X\right]_l \{a_n^+\} \\ \{s_{n'}^V\} &= \sum_{n=0}^{N} \left[CS_{n'n}^V\right]_l \{a_n^-\} \\ \{s_{n'}^W\} &= \sum_{n=0}^{N} \left[CS_{n'n}^W\right]_l \{a_n^-\} \end{aligned} \tag{63}$$

$0 \leq n' \leq N + 4$. The "*conversion*" arrays depend only on l and are precomputed. Their construction is related to the coefficients β_{ni} that are determined through elementary properties of Chebyshev polynomials.

SEMI-DISCRETE EQAUTIONS

Equation (19) is semi-discretized by utilizing the orthogonality between the basis and test functions. With the expressions for $\boldsymbol{u}$, $\boldsymbol{\psi}$ and $\boldsymbol{F}$ from (50)-(56) substituted in (19), and further using the orthogonality of VSHs, we obtain, for every pair (l,m), two uncoupled sets ("+" and "−") of $(N+1)$ semi-discrete equations

$$\sum_{n=0}^{N}\left(\frac{da^-_{nlm}}{dt}\int_{R_i}^{R_o} h^-_n\, g^-_{n'}\, r^2\, dr - \frac{1}{Re}a^-_{nlm}\int_{R_i}^{R_o} L_l(h^-_n)\, g^-_{n'}\, r^2\, dr\right) = \sum_{n=0}^{N_d} f^X_{nlm}\int_{R_i}^{R_o} T_n\, g^-_{n'}\, dr - \left(\int_{R_i}^{R_o}\left[\dot{\Lambda}^0_m(t)T_0(\xi)+\dot{\Lambda}^1_m(t)T_1(\xi)\right]g^-_{n'}(r)\, r^2\, dr + \frac{1}{Re}2\left[K\Lambda^1_m(t)-\Lambda^0_m(t)\right]\int_{R_i}^{R_o} g^-_{n'}(r)\, dr\right)\delta_{l1} \quad (64)$$

and

$$\sum_{n=0}^{N}\left(\frac{da^+_{nlm}}{dt}\int_{R_i}^{R_o}\left[h^{+V}_{nl}\, g^{+V}_{n'l} + h^{+W}_{nl}\, g^{+W}_{n'l}\right] r^2\, dr - \frac{1}{Re}a^+_{nlm}\int_{R_i}^{R_o} L_{l+1}(h^{+V}_{nl})\, g^{+V}_{n'l}\, r^2\, dr - \frac{1}{Re}a^+_{nlm}\int_{R_i}^{R_o} L_{l-1}(h^{+W}_{nl})\, g^{+W}_{n'l}\, r^2\, dr\right) = \sum_{n=0}^{N_d}\int_{R_i}^{R_o}\left[f^V_{nlm}T_n\, g^{+V}_{n'l} + f^W_{nlm}T_n\, g^{+W}_{n'l}\right] r^2\, dr \quad (65)$$

where $0 \le n' \le N$ and

$$L_l \equiv \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}.$$

With the following definitions

$$\begin{aligned}
\mathcal{A}^-_{n'n} &= \int_{R_i}^{R_o} h^-_n\, g^-_{n'}\, r^2\, dr\\
\mathcal{B}^-_{n'n} &= \int_{R_i}^{R_o} L_l(h^-_n)\, g^-_{n'}\, r^2\, dr\\
\mathcal{A}^+_{n'n} &= \int_{R_i}^{R_o}\left[h^{+V}_{nl}\, g^{+V}_{n'l} + h^{+W}_{nl}\, g^{+W}_{n'l}\right] r^2\, dr\\
\mathcal{B}^+_{n'n} &= \int_{R_i}^{R_o}\left[L_{l+1}(h^{+V}_{nl})\, g^{+V}_{n'l} + L_{l-1}(h^{+W}_{nl})\, g^{+W}_{n'l}\right] r^2\, dr\\
\mathcal{F}^X_{n'n} &= \int_{R_i}^{R_o} T_n\, g^-_{n'}\, dr\\
\mathcal{F}^V_{n'n} &= \int_{R_i}^{R_o} T_n\, g^{+V}_{n'l}\, dr\\
\mathcal{F}^W_{n'n} &= \int_{R_i}^{R_o} T_n\, g^{+W}_{n'l}\, dr\\
T^{bc^-}_{n'}(t) &= \int_{R_i}^{R_o}\left[\dot{\Lambda}^0_m(t)T_0(\xi)+\dot{\Lambda}^1_m(t)T_1(\xi)\right]g^-_{n'}(r)\, r^2\, dr\\
V^{bc^-}_{n'}(t) &= 2\left[K\Lambda^1_m(t)-\Lambda^0_m(t)\right]\int_{R_i}^{R_o} g^-_{n'}(r)\, dr
\end{aligned}$$

equations (64) and (65), for every pair (l,m), are compactly written as

$$\sum_{n=0}^{N}\left(\left[\mathcal{A}^-_{n'n}\right]\cdot\{\dot{a}^-_n\} - \frac{1}{Re}\left[\mathcal{B}^-_{n'n}\right]\cdot\{a^-_n\}\right) = \sum_{n=0}^{N+4}\left(\left[\mathcal{F}^X_{n'n}\right]\cdot\{f^X_n\}\right) - \{T^{bc^-}_{n'}\}\,\delta_{1l} + \frac{1}{Re}\{V^{bc^-}_{n'}\}\,\delta_{1l} \quad (66)$$

and

$$\sum_{n=0}^{N}\left(\left[\mathcal{A}^+_{n'n}\right]\cdot\{\dot{a}^+_n\} - \frac{1}{Re}\left[\mathcal{B}^+_{n'n}\right]\cdot\{a^+_n\}\right) = \sum_{n=0}^{N+4}\left(\left[\mathcal{F}^V_{n'n}\right]\cdot\{f^V_n\} + \left[\mathcal{F}^W_{n'n}\right]\cdot\{f^W_n\}\right) \quad (67)$$

These arrays also depend only on l and are precomputed. Their construction utilizes the orthogonality of Chebyshev polynomials and is done in the following manner. As was mentioned before, the radial basis and test functions can be generally expressed as

$$x_{nl}(\xi) = \sum_{j=-4}^{4} \beta_{nlj} T_{n+j}(\xi)$$

or, by replacing j with $p = n + j$,

$$x_{nl}(\xi) = \sum_{p=n-4}^{n+4} \beta_{nl(p-n)} T_p(\xi)$$

Therefore, the arrays can now be generally expressed as

$$[\mathcal{X}_{n'n}]_l = \int_{-1}^{1} \left(\sum_{j=n-4}^{n+4} \beta_{nl(j-n)} T_j(\xi) \right) \left(\sum_{i=n-4}^{n+4} \gamma_{n'l(i-n')}\, T_i(\xi) \right) \frac{d\xi}{\sqrt{1-\xi^2}}. \tag{68}$$

Upon using the orthogonality of Chebyshev polynomials, we get

$$[\mathcal{X}_{n'n}]_l = \sum_{j=n-4}^{n+4} \sum_{i=n'-4}^{n'+4} \beta_{nl(j-n)} \gamma_{n'l(i-n')} c_j \frac{\pi}{2} \delta_{ji} \tag{69}$$

which can be further simplified to

$$[\mathcal{X}_{n'n}]_l = \sum_{j=n-4}^{n+4} \beta_{nl(j-n)} \gamma_{n'l(j-n')} c_j \frac{\pi}{2}. \tag{70}$$

Thus again, the construction of these arrays also boils down to the determinaltion of β_{ni} and γ_{ni}.

DISCRETE EQUATIONS

The time discretization of the ordinary differential equation (59) is done through standard finite difference schemes. For the viscous term, a second-order Crank-Nicholson scheme is used. The non-linear term is treated explicitly through the second-order Adams-Bashforth scheme. Thus, for every pair (l, m), the ordinary differential equations (56) and (57) are transformed into the following discrete equations

$$\left[\mathcal{A}^{\pm} - \frac{\Delta t}{2Re} \mathcal{B}^{\pm} \right] \{a_n^{\pm}\}^{j+1} = \left[\mathcal{A}^{\pm} + \frac{\Delta t}{2Re} \mathcal{B}^{\pm} \right] \{a_n^{\pm}\}^{j} + \frac{3\Delta t}{2} \{\mathcal{R}^{\pm}\}^{j} - \frac{\Delta t}{2} \{\mathcal{R}^{\pm}\}^{j-1} \tag{71}$$

with

$$\begin{aligned} \mathcal{R}^{+} &\equiv \mathcal{F}^{+} \\ \mathcal{R}^{-} &\equiv \mathcal{F}^{-} - T^{bc^{-}} \delta_{l1} + \frac{1}{Re} V^{bc^{-}} \delta_{l1}, \end{aligned}$$

where j denotes the time-step. For the first time-step, a forward Euler scheme, instead of Adam-Bashforth scheme, is used fro the non-linear term. A numerical program (implementable in FORTRAN) is described below. Before doing so, a few computationaly relevant points ought to be mentioned. First, the coefficients $a_{nlm}^{\pm}$ show indicial symmetry, i.e.,

$$a_{nl(-m)}^{\pm} = (-1)^{m+1} (a_{nlm}^{\pm})^{*} \tag{72}$$

where "$*$" denotes complex conjugate. Therefore, only the non-negative m coefficients need to be stored and marched in time. Second, since the arrays in equation () depend only on l, a single matrix inversion can be done for $M + 1$ equations together.

NUMERICAL PROGRAM

Arrays:

- `complex, dimension(0:Nd,1:L,-M:M+1) ::  F1, F2, F3`
  these arrays hold $f^X_{lm}(\xi_n), f^V_{lm}(\xi_n), f^W_{lm}(\xi_n)$ computed at the end of j^{th} time-step
- `complex, dimension(0:max(Nd,Ld),-M:M+1) ::  A, B, C, D, E, F`
- `complex, dimension(0:N,0:M) ::  Am, Ap`
- `complex, dimension(1:L,0:N,0:M) ::  Fm, Fp`
  these arrays hold $\{\mathcal{Q}_{n'm}\}_l = \left(\sum_{n=0}^{N}\left[\mathcal{A}^{\pm}_{n'n} + (\Delta t/2Re)\mathcal{B}^{\pm}_{n'n}\right]_l \{a^{\pm}_{nlm}\}^j + \{\mathcal{R}^{\pm}_{n'm}\}^{j-1}_l\right)$ computed in the j^{th} time-step.
- `complex, dimension(0:N,0:M) ::  T, V`
  arrays corresponding to the contribution of the boundary condition terms $\mathcal{T}^{bc^-}_{n'm}, \mathcal{V}^{bc^-}_{n'm}$.
- `real, dimension(1:L,0:N,0:N) ::  P1m, P1p, P2m, P2p`
  these are the precomputed arrays $\left[\mathcal{A}^{\pm}_{n'n} + (\Delta t/2Re)\mathcal{B}^{\pm}_{n'n}\right]_l$ and $\left[\mathcal{A}^{\pm}_{n'n} - (\Delta t/2Re)\mathcal{B}^{\pm}_{n'n}\right]_l$
- `real, dimension(1:L,0:N,0:N+4) ::  NLx, NLv, NLw`
  these arrays correspond to $\left[\mathcal{F}^X_{n'n}\right]_l, \left[\mathcal{F}^V_{n'n}\right]_l, \left[\mathcal{F}^W_{n'n}\right]_l$
- `real, dimension(1:L,0:N+4,0:N) ::  CUx, CUv, CUw, CSx, CSv, CSw`
  conversion arrays to corresponding to $\left[CU^X_{n'n}\right]_l, \left[CU^V_{n'n}\right]_l, \left[CU^W_{n'n}\right]_l, \left[CS^X_{n'n}\right]_l \left[CS^V_{n'n}\right]_l \left[CS^W_{n'n}\right]_l$

$(j+1)^{th}$ `TIME-STEP`
`DO l = 1, L`

1. Copy VSH transformed coefficients $f^X_{lm}(\xi_n), f^V_{lm}(\xi_n), f^W_{lm}(\xi_n)$ (in the (n,m)-"plane") from `F1,F2,F3` to `D,E,F`.
2. For every $m\,(0 \le m \le min(l,M))$, backward Chebyshev transform `D(:,m), E(:,m), F(:,m)`
3. if `(l = 1)` then `Am(n,m) = T(n,m) + V(n,m)`
4. For every $(n,m)\,(0 \le n \le N, 0 \le m \le M)$ compute $[\mathcal{F}_{n'n}]_l \{f_{nlm}\}$ and add it to $\{\mathcal{Q}_{n'm}\}_l$ stored in `Fm, Fp`, i.e.,
   (a) `Ap(n,m) =` $\sum_{i=0}^{N+4}$ `(NLv(n,i)*E(i,m) + NLw(n,i)*F(i,m))`
   (b) `Am(n,m) = Am(n,m) +` $\sum_{i=0}^{N+4}$ `NLx(n,i)*D(i,m)`
   (c) `Fm(l,n,m) = Fm(l,n,m) + (3Δt/2)*Am(n,m)`
   (d) `Fp(l,n,m) = Fp(l,n,m) + (3Δt/2)*Ap(n,m)`
5. For every $m\,(0 \le m \le min(l,M))$, solve the matrix equations
   `[P1m(l,:,:)]Fm(l,:,m) = Fm(l,:,m)`
   `[P1m(l,:,:)]Fp(l,:,m) = Fp(l,:,m)`
   to obtain new $a^{\pm}_{nlm}$ in `Fp, Fm`
6. For every (n,m), $(0 \le n \le N, 0 \le m \le M)$, compute $\{\mathcal{R}_{n'm}\}^{j+1}$ and store it in `Am, Ap`
   (a) `Am(n,m) =` $\sum_{i=0}^{N}$ `P2m(l,n,i)*Fm(i,m) - (Δt/2)*Am(n,m)`
   (b) `Ap(n,m) =` $\sum_{i=0}^{N}$ `P2p(l,n,i)*Fp(i,m) - (Δt/2)*Ap(n,m)`
7. For every $(n,m)\,(0 \le n \le N+4, 0 \le m \le M)$, compute coefficients of velocity and vorticity in standard Chebyshev representation
   (a) `A(n,m) =` $\sum_{i=0}^{N}$ `CUx(n,i)*Fm(i,m)`
   (b) `B(n,m) =` $\sum_{i=0}^{N}$ `CUv(n,i)*Fp(i,m)`
   (c) `C(n,m) =` $\sum_{i=0}^{N}$ `CUw(n,i)*Fp(i,m)`
   (d) `D(n,m) =` $\sum_{i=0}^{N}$ `CSx(n,i)*Fp(i,m)`

(e) `E(n,m) =` $\sum_{i=0}^{N}$ `CSv(n,i)*Fm(i,m)`

(f) `F(n,m) =` $\sum_{i=0}^{N}$ `CSw(n,i)*Fm(i,m)`

8. For every $m\,(0 \leq m \leq min(l, M))$, forward Chebyshev transform `A,B,C, D,E,F` to obtain $u_{lm}^{X}(\xi_n), u_{lm}^{V}(\xi_n), u_{lm}^{w}(\xi_n),\ s_{lm}^{X}(\xi_n), s_{lm}^{V}(\xi_n), s_{lm}^{W}(\xi_n)$ and store it in `F1,F2,F3`

9. `Fm = Am, Fp = Ap`

`END DO`

`DO n = 0,Nd`

1. Copy the coefficients $u_{lm}^{X}(\xi_n), u_{lm}^{V}(\xi_n), u_{lm}^{w}(\xi_n),\ s_{lm}^{X}(\xi_n), s_{lm}^{V}(\xi_n), s_{lm}^{W}(\xi_n)$ (in the (l, m)-“plane”) from `F1,F2,F3` to `A,B,C, D,E,F` (set the coefficients with $L \leq l \leq L_d, M \leq m \leq M_d$ equal to zero)

2. Forward VSH transform `A,B,C, D,E,F` to physical space

3. Compute the product $r\boldsymbol{u} \times (r\nabla \times \boldsymbol{u})$ and store in `D,E,F`

4. For every m, backward VSH transfrom `D,E,F` and transfer to `F1,F2,F3`

`END DO`
`END OF TIME-STEP`

CONCLUSION

The presented method does not assume any sort of symmetry. Although, the choice of basis functions used to expand velocity and test function is greatly influenced by geometry and boundary conditions, there are no additional constraints imposed on the velocity field. This method is not just limited to bounded domains. With appropriate choice of basis functions, it can be used to study semi-infinite and infinite flows. Furthermore, it is not very difficult to extend the application of this method to other curvilinear orthogonal coordinate systems.

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