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Spurious Modes in Spectral Collocation Methods with Two Non-periodic Directions

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Abstract

Collocation implementation of the Kleiser-Schumann's method in geometries with two non-periodic directions is shown to suffer from three spurious modes – *line, column* and *checkerboard* – contaminating the computed pressure field. The *corner* spurious modes are also present but they do not affect evaluation of pressure related quantities. A simple methodology in the inversion of the influence matrix will efficiently filter out these spurious modes.

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1. Introduction

Most existing numerical solutions of incompressible Navier-Stokes equations in three dimensions employ the primitive-variable formulation. Here, the velocity field and pressure can not be approximated independently and must satisfy a compatibility condition. Approximating both velocity and pressure by polynomials of the same degree will result in some spurious modes for the pressure [1]. In a spectral collocation implementation, these spurious modes can be characterized as the spurious components of the pressure field whose discrete gradient at the interior collocation points, where discretized momentum equations are satisfied, is zero. Such pressure components have no effect on velocity and are therefore left uncontrolled by the discretized governing equations.

Existence of spurious pressure modes in a spectral simulation was first pointed out by Morchoisne [2]. In coupled spectral implementations where the continuity equation is discretized directly, theoretical analysis of the spurious modes is on a firm footing [1]. When a non-staggered grid is employed it has been shown that a fully periodic problem has no spurious modes, discounting the arbitrariness of the mean value of pressure in an incompressible flow. In a flow with one non-periodic direction pressure has one spurious mode, and problems with two non-periodic directions have seven (1-*line*, 1-*column*, 1-*checkerboard* and 4-*corner*) spurious modes [1,3]. These results have been shown to apply to the following spectral implementations: Galerkin Legendre, Legendre tau, Galerkin Chebyshev, Chebyshev tau and Chebyshev collocation with Gauss-Lobatto points. In a collocation implementation, the spurious modes can be avoided with an appropriately staggered mesh for velocity and pressure. Montigny-Rannou and Morchoisne [4] have recently described an algorithm for the two non-periodic problem on a half-staggered grid which involves only one (*checkerboard*) spurious mode. The spurious modes can be completely avoided in a two non-periodic problem with a fully-staggered mesh [5, 6].

A second class of numerical algorithms avoids direct solution of the continuity equation by solving a Poisson equation for pressure [1]. The time-split implementation [7] is the simplest of them all but it suffers from non-zero boundary divergence, non-zero slip velocity and time-splitting errors. Kleiser-Schumann's influence matrix method can be used to enforce zero boundary divergence and no-slip condition [8,9]. A partial implementation of the influence matrix is simpler, but will result in small but non-zero interior divergence [10]. A full implementation of the Kleiser-Schumann's method with *tau* (or *collocation*) correction enforces interior zero divergence as well. Here we identify the spurious modes in the collocation implementation of the Kleiser-Schumann method [8, 9, 11] with tau correction for a problem with two non-periodic directions to be the *line, column, checkerboard* and *corner* modes. A simple correction procedure which will automatically filter these spurious modes is obtained. This correction procedure is applied in the simulation of a turbulent square duct flow [11] and is found to be very effective in eliminating spurious modes.

2. Spurious Modes for Kleiser-Schumann's Method

The full implementation of the Kleiser-Schumann's method with *collocation* correction can be given by the following equations and boundary conditions:

$$\begin{aligned}
\nabla^2 p &= -\nabla\cdot(\boldsymbol{NL}) + \nabla\cdot\boldsymbol{B} && \text{in } \boldsymbol{\Omega} \\
\frac{\partial \boldsymbol{V}}{\partial t} + \boldsymbol{NL} &= -\nabla p + \frac{1}{\mathrm{Re}}\nabla^2\boldsymbol{V} + \boldsymbol{B} && \text{in } \boldsymbol{\Omega}, \partial\boldsymbol{\Omega} \\
\boldsymbol{V} &= \boldsymbol{V}_b && \text{on } \partial\boldsymbol{\Omega} \\
\nabla\cdot\boldsymbol{V} &= 0 && \text{on } \partial\boldsymbol{\Omega} \\
\boldsymbol{B} &= 0 && \text{in } \boldsymbol{\Omega}
\end{aligned} \tag{1a–1e}$$

where $\boldsymbol{NL}$ is the nonlinear term in the Navier-Stokes equation and $\boldsymbol{V}_b$ is the velocity boundary condition. The above equations and boundary conditions are in their discretized form, therefore the symbols $\nabla, \nabla\cdot$ and ∇^2 represent discrete gradient, divergence and Laplacian operators, and $\boldsymbol{\Omega}$ and $\partial\boldsymbol{\Omega}$ represent interior and boundary collocation points. Since the momentum equation is satisfied only in the interior, $\boldsymbol{B}$ represents the boundary momentum residual and is nonzero only on the boundary. Combining equation (1a) and the discrete divergence of equation (1b) one obtains $\frac{\partial \nabla\cdot\boldsymbol{V}}{\partial t} = \frac{1}{\mathrm{Re}}\nabla^2(\nabla\cdot\boldsymbol{V})$ in $\boldsymbol{\Omega}$, provided the discrete divergence of the discrete gradient operator is identically equal to the discrete Laplacian operator. The above equation for the velocity divergence along with the boundary condition given by equation 1d, results in a divergence free velocity field both in the interior and on the boundary.

By definition, each spurious mode is a valid solution to the discretized governing equations and appropriate boundary conditions. The spurious modes have a non-zero contribution to pressure but have no effect on velocity, therefore $\boldsymbol{V}_{sp} = 0$, where subscript "sp" stands for the spurious mode. The spurious pressure components therefore satisfy

$$\nabla^2 p_{sp} = \nabla \cdot \boldsymbol{B}_{sp} \qquad \text{in } \Omega$$

$$0 = -\nabla p_{sp} + \boldsymbol{B}_{sp} \qquad \text{in } \Omega, \partial\Omega \tag{2a–2c}$$

$$\boldsymbol{B}_{sp} = 0 \qquad \text{in } \Omega$$

where $\boldsymbol{B}_{sp}$ is the corresponding spurious boundary momentum residual. Any non-trivial solution to the above linear equations represents a spurious mode, which when added to the true solution will still satisfy the discretized Navier-Stokes equations and boundary conditions.

Eight solutions to the above equations can be identified. First of which is the non-spurious solution, p_{sp} = constant and $\boldsymbol{B}_{sp} = 0$, which indicates that pressure is evaluated only up to an arbitrary additive constant in incompressible flows. The first two spurious modes are the *line* and *column* modes

$$P_{sp} = T_{Nx}(x)\ , \quad B_{1sp} = \begin{cases} (\pm\ 1)^{Nx}(Nx)^2 & \text{at } x = \pm\ 1 \\ 0 & \text{otherwise} \end{cases}\ , \quad B_{2sp} = B_{3sp} = 0$$

$$P_{sp} = T_{Ny}(y)\ , \quad B_{2sp} = \begin{cases} (\pm\ 1)^{Ny}(Ny)^2 & \text{at } y = \pm\ 1 \\ 0 & \text{otherwise} \end{cases}\ , \quad B_{1sp} = B_{3sp} = 0 \tag{3}$$

Here $(Nx+1)$ and $(Ny+1)$ are the number of points along the non-periodic Chebyshev directions and the third direction is at most periodic. B_1, B_2 and B_3 are the three components of the boundary momentum residual and only the normal component is nonzero. T_{Nx} and T_{Ny} are Chebyshev polynomials of the highest degree along x and y. The third spurious mode is the *checkerboard* mode, with

$$P_{sp} = T_{Nx}(x)\ T_{Ny}(y)\ , \quad B_{1sp} = \begin{cases} (\pm\ 1)^{Nx}(Nx)^2\ T_{Ny}(y) & \text{at } x = \pm\ 1 \\ 0 & \text{otherwise} \end{cases}$$

$$B_{2sp} = \begin{cases} (\pm\ 1)^{Ny}(Ny)^2\ T_{Nx}(x) & \text{at } y = \pm\ 1 \\ 0 & \text{otherwise} \end{cases}\ , \qquad B_{3sp} = 0 \tag{4}$$

These three spurious modes have no variation in the periodic z direction and therefore contaminate only the zero$^{\text{th}}$ mode along the z direction. The other four spurious modes are the *corner* modes and each of them can have arbitrary variation along the z direction. For example, let $f_{1,1}(z)$ be the arbitrary variation along the x=1, y=1 corner. Then the *corner* mode corresponding to this corner can now be written as

$$P_{sp} = \begin{cases} f_{1,1}(z) & \text{at } x = y = 1 \\ 0 & \text{otherwise} \end{cases}, \quad B_{1sp} = \begin{cases} f_{1,1}(z)\ D_{Nx}(x) & \text{at } y = +1 \\ 0 & \text{otherwise} \end{cases}$$

$$B_{2sp} = \begin{cases} f_{1,1}(z)\ D_{Ny}(y) & \text{at } x = +1 \\ 0 & \text{otherwise} \end{cases}, \quad B_{3sp} = \begin{cases} \dfrac{df_{1,1}}{dz} & \text{at } x = y = 1 \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

where $D_{Nx}(x)$ is the discrete derivative of the polynomial which collocates to zero at all points except at x=1. The *corner* modes for the other three corners can be written similarly. The *corner* spurious modes simply reflect the fact that in a collocation implementation the pressure along the four corner-lines never enter into the computation and therefore their values remain unspecified. This arbitrariness associated with the corner pressure values is relatively innocuous, since they are not required in computing pressure related quantities of interest. On the other hand, the other three spurious modes are buried in the numerically computed pressure and need to be filtered out.

3. Filtering Procedure

Implementation of the Kleiser-Schumann's method involves the construction of an influence matrix. The solution of the pressure Poisson equation (equation 1a) requires the knowledge of pressure boundary conditions (p_b) and boundary momentum residuals ($\boldsymbol{B_b}$) at the ($2N_x$+$2N_y$–4) points, excluding the corner points. Note that in the three, *line, column* and *checkerboard* modes only the normal component of the boundary momentum residual is nonzero. In essence, a total of ($4N_x$+$4N_y$–8) unknown boundary pressure and normal momentum residuals are required in evaluating the pressure field. These unknowns are evaluated by requiring that continuity and normal momentum (with the residual) are satisfied at the boundary points excluding the corner points. This provides the necessary ($4N_x$+$4N_y$–8) linear equations for the unknown quantities. These equations can be cast into the following matrix form, $\underline{\underline{A}}\ \underline{x} = \underline{R}$, where $\underline{\underline{A}}$ is the influence matrix, $\underline{x}$ is the unknown vector of boundary pressure and normal momentum residual and $\underline{R}$ is the right hand side. In a three-dimensional problem, a Fourier transform along the periodic z direction will result in one influence matrix for each Fourier wavenumber k_z. Invertibility of the influence matrix is closely related to the presence of spurious modes. In particular the influence matrix corresponding to k_z=0 suffers from the *constant, line, column* and *checkerboard* modes. This influence matrix therefore has four zero eigenvalues. In the numerical computation of a turbulent square duct flow it was observed that only for k_z=0 were four eigenvalues of the influence matrix of the order 10^{-12}, while the lowest of all other eigenvalues were around 10^{-6}. The eigenvectors corresponding to these eigenvalues are the corresponding spurious boundary pressure and normal component of the momentum residual.

As suggested by Tuckerman [9], the non-invertibility of the influence matrix can be easily overcome by constructing a related matrix $\underline{\underline{A'}} = \underline{\underline{M}}\ \underline{\underline{\lambda'}}\ \underline{\underline{M}}^{-1}$, where $\underline{\underline{M}}$ and $\underline{\underline{M}}^{-1}$ are the eigenvector matrix of the original influence matrix and its inverse, respectively, and $\underline{\underline{\lambda}}'$ is a diagonal matrix with the eigenvalues along the diagonal and with the zero eigenvalues replaced by some non-zero constant. The influence matrix now becomes invertible, i.e., $\underline{\underline{A'}}^{-1} = \underline{\underline{M}}\ \underline{\underline{1/\lambda'}}\ \underline{\underline{M}}^{-1}$, and the resulting pressure and boundary momentum residuals yield a divergence-free flow field independent of the constant that replaces the zero eigenvalue. Let the p^{th} eigenvalue of the original influence matrix be zero and be replaced by a constant c_p. Let the corresponding p^{th} eigenvector be M_{ip}, which is a vector of boundary pressures and momentum residuals corresponding to a linear combination of the spurious modes. Contribution of this p^{th} mode to the unknown vector x_i is then $\frac{M_{ip} b_p}{c_p}$, where b_p is the projection of the right hand side along the eigenvectors, given by $M_{pj}^{-1}\ R_j$. One simple way to filter the four spurious modes will then be to set the arbitrary constant c_p to be infinity. In other words, in the evaluation of $\underline{\underline{A'}}^{-1}$, one over the zero eigenvalue is replaced by zero. This filtering procedure was implemented in the computation of turbulent flow in a square duct [11] and it essentially removed all high frequency checkerboard type oscillations. It should be pointed out that such oscillations can be observed in the $k_z \neq 0$ modes as well, especially at high Reynolds numbers when resolution is only marginal. These oscillations are not due to the spurious modes, but are controlled energy in the high wavenumber modes.

4. Spurious Modes in Partial and Time-Split Methods

Spurious modes for the partial implementation of the Kleiser-Schumann's method without the *collocation* correction can be analyzed in similar fashion. The spurious modes satisfy the following equations.

$$\nabla^2 p_{sp} = 0 \qquad \text{in } \Omega$$

$$0 = -\nabla p_{sp} + \boldsymbol{B}_{sp} \qquad \text{in } \Omega, \partial\Omega \qquad \text{(6a–6c)}$$

$$\boldsymbol{B}_{sp} = 0 \qquad \text{in } \Omega$$

It can be easily seen that the only admissible solution for the above set of equations is the non-spurious *constant* mode and there are no spurious modes present. This is confirmed in the numerical simulation by observing that the influence matrix for the k_z=0 mode has only one zero eigenvalue and the corresponding constant mean pressure can be set to zero by replacing the zero eigenvalue by infinity.

Spurious modes in the time split implementation will depend on the exact boundary conditions employed for the intermediate star-level velocities ($\boldsymbol{V}^*$) and the pressure Poisson equation. Following Streett and Hussaini [7], if we employ $\left[(2\nabla p(t) - \nabla p(t - \delta t)) \cdot \boldsymbol{\tau}\right]$ as the boundary condition for the tangential components of the intermediate star-level velocity, zero penetration for the normal velocity component and zero Neumann boundary condition for the pressure, then we have the following equations satisfied by the spurious modes:

$$\boldsymbol{V}^*_{sp} = \Delta t \, \nabla p_{sp} \qquad \text{in } \Omega$$

$$\nabla^2 \boldsymbol{V}^*_{sp} = \frac{2Re}{\Delta t} \boldsymbol{V}^*_{sp} \qquad \text{in } \Omega$$

$$\boldsymbol{V}^*_{sp} \cdot \boldsymbol{\eta} = \nabla p_{sp} \cdot \boldsymbol{\eta} = 0 \qquad \text{in } \partial\Omega \qquad \text{(7a–7d)}$$

$$\boldsymbol{V}^*_{sp} \cdot \boldsymbol{\tau} = \left(2\nabla p_{sp}(t) - \nabla p_{sp}(t - \delta t)\right) \cdot \boldsymbol{\tau} \qquad \text{in } \partial\Omega$$

where $\boldsymbol{\eta}$ and $\boldsymbol{\tau}$ are direction normal and tangential to the boundary. The analysis of the spurious modes is more complicated and also depends on the initial tangential pressure gradients on the boundary. With careful choice of initial conditions, the no penetration and pure Neumann boundary conditions will guarantee no spurious components.

5. Conclusion

Collocation implementation of the Kleiser-Schumann's method in geometries with two non-periodic directions have three spurious modes – *line, column* and *checkerboard* – contaminating the computed pressure field. The *corner* spurious modes are also present but they do not affect evaluation of pressure related quantities. The three spurious modes can be easily filtered out by replacing the zero eigenvalues of the influence matrix with infinity before solving for the unknown boundary pressure and momentum residuals. Partial implementation of the Kleiser-schumann's method without *collocation* correction admits no spurious modes. Spurious modes can also be avoided in time-split implementations.

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