Nonlinear dynamics for the 3D ideal viscous gas flow over the cylinder

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Abstract. The system of governing equations for the dynamics of the compressible viscous ideal gas is considered in the 3D bounded domain with the inflow and outflow boundary conditions. The cylinder is located in the domain. Such problem is simulated using the high order WENO-scheme for inviscid part of the equations and using 4-th order central approximation for the viscous tensor part with the third order temporal discretization.

The method of Proper Orthogonal Decomposition (POD) is applied to the problem at hand in order to extract the most active nodes. Cascades of bifurcations of periodic orbits and invariant tori are found that correspond to the excitation in different POD modes. The approximation of the reduced order model is analyzed and it is shown that one cannot make parameter extrapolations for the reduced order model to capture the same dynamics as is observed in the original full size model.

1. Introduction
The problem of the laminar turbulent transition is a classical problem, where many different methods and models are used. In this study we focus on the application of the dynamical system approach coupled with the Proper Orthogonal Decomposition (POD). The analysis of transitional regimes in a flow over a cylinder is a problem that was tackled by many different approaches and methods. In this study we focus on the dynamical system approach. First we present the overview of the problem at hand. Most cases are considered either for incompressible or almost incompressible flows. An experimental research was conducted in [1], where it was found that the dynamics of fluctuating velocity can be described by the Landau equation in the vicinity of the critical Reynolds number. A Hopf bifurcation was confirmed that resulted in the birth of the limit stable cycle. Classical results of the cylinder flow transition to turbulence process are reviewed in [2] in terms of experimental data. It is shown that the primary instabilities are 2D in the initial stage of the transition. It is shown that for the Reynolds number below 49 the solution is a laminar steady state. The laminar unsteady state is observed for the Reynolds numbers between 50 and, approximately, 140 – 190. A 3D structures appear starting from Reynolds around 190 and continue to evolve into turbulence. The following scenario is observed in terms of the Reynolds number (R): as R increases, the wake velocity fluctuations indicate a cascade of period-doubling bifurcations, which create a chaotic state in the flow at around R=500. However some experimental and numerical data doesn’t support the scenario of period doubling for domains larger than 1.5 cylinder diameters, for example [3]. For further overview of the modern results refer to [4]. The direct numerical simulations of cross-flow over
a circular cylinder are performed for the Reynolds number 100, 220, 300, 800 and 1575. It is shown that the initial instability of cylinder wakes is transformed from 2D to 3D instabilities that spawn two different solutions. The conclusion is supported using POD analysis with the comparison of active POD modes (i.e. flow expansion in terms of the optimal energy basis) for different Reynolds numbers. The problem of the dynamics in the rotating cylinder problem was considered in [5]. Three codimension-two bifurcation points are identified, namely a Takens–Bogdanov, a cusp and generalized Hopf, which are closely related to qualitative changes in orbit dynamics. The chaotic dynamics for square cylinder (box) is considered in [6] for 2D flow. The route to chaos is found to be formed by two Hopf bifurcations that form two-dimensional torus at the Reynolds number around 210, after which the phase locking is identified at around 315. Frequency locking is observed starting at 325 to 375 (in terms of the Reynolds number), the chaotic solution is found at R around 500. Interesting results in the paper [7] for the Mode C instabilities (the Mode C wake instability is generated by placing a small wire in the near wake of a main circular cylinder), however we don’t focus on alternative setups.

One can observe that the analysis of dynamics for the compressible flow, where compressible effects cannot be ignored, is not considered. This paper focuses on two primary aspects:

- investigation of the transition to chaotic regime from the dynamical systems point of view for compressible subsonic flow around a cylinder;
- analysis of POD approach and its utilization as a reduced order dynamical system.

The paper has the following structure. First, the governing equations are formulated and the used numerical method is laid out. The numerical method is only given in brief. Next, the method of analysis is presented that includes the Poincare section methods and the description of the applied POD approach. Next the results are outlined and discussed. Observe, that the results presented in the paper are preliminary results and further research is expected.

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2. Governing equations, numerical method
This section gives a brief description of the governing equations, numerical method and the method of analysis used in this study.

2.1. Governing equations
We are considering conservation laws for viscous gas dynamics. This system can be written in the following conservative form [8]:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} [\rho u_j] &= 0, \\
\frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_j} [\rho u_i u_j + p \delta_{ij} - \tau_{ij}] &= 0, \quad i, j, k = \{1, 2, 3\}; \\
\rho E &= \frac{1}{2} \rho u^2 + \rho e, \\
p &= (\gamma - 1) (E - \frac{1}{2} \rho u^2).
\end{align*}
\]

(1)

Here we are considering some bounded domain $\Omega \subset \mathbb{R}^3$ with boundary $\partial \Omega$, scalar functions $f$ are defined as $f : \Omega \times [0, T] \to \mathbb{R}$, vector-functions $\mathbf{f}$ are defined as $\mathbf{f} : \Omega \times [0, T] \to \mathbb{R}^3$, where $T$ is some defined finite time. Then $\rho E$ is a scalar function of the full gas energy; $\gamma$ is the adiabatic index (value 1.4 is used for calculations); $p$ is the pressure scalar function; $\mathbf{u}$ is a gas velocity vector function; $\rho$ is a scalar function of gas
density. Assuming Einstein summation rule. We also assume that the gas is Newtonian with the following viscous tensor:

$$\tau_{ij} = 2\mu S_{ij},$$

where $\mu$ is a dynamic gas viscosity and strain rate tensor is defined as:

$$S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k}. \quad (3)$$

Please note that we ignore the second coefficient of viscosity due to complexity. We use integral form of (1) for problems that may have discontinuous solutions. We use the main bifurcation parameter that is considered in the paper - the Reynolds number. It is defined as:

$$R = \frac{L_C ||u_C|| \rho_C}{\mu}, \quad (4)$$

where $L_C$ is the characteristic length scale of the problem, $||u_C||$ is the norm of the characteristic velocity vector, $\rho_C$ is a characteristic density. With this in mind, we can rewrite (2) as follows:

$$\tau_{ij} = \frac{2}{R} S_{ij}. \quad (5)$$

We will use (2) if we use the term ”viscosity coefficient” and we use (5) if we use the term ”Reynolds number” which is used as the ”parameter” in the bifurcation study. All units are non-dimensional w.r.t the cylinder diameter, far field velocity and density are taken as characteristic length, velocity and density respectively.

The domain size is $18 \times 1 \times 6$ in x,y and z directions, respectively. The cylinder of radius 0.5 is considered in the domain with the center axis line $x = 2, z = 3$. The cylinder generatrix is parallel to the y direction ort. The wall boundary condition is set on the surface of the cylinder with zero velocity (no-slip condition). Other boundary conditions are given as follows: outflow boundary condition on the plane $x = 18$ and inflow boundary conditions on the plane $x = 0$. The inflow boundary sets the far field values $\rho_0 = 1.24, u_0 = (1, 0, 0)^T$, other flow parameters are selected such, that the inflow Mach number is 0.5. The boundary conditions on the $y = 0$ and $y = 1$ are periodic and boundaries on $z = 0$ and $z = 6$ planes are posed as symmetric (free slip condition). The initial conditions for the first run (the lowest value of the parameter) are set to the uniform flow in the domain with the creeping flow (pure diffusive flow is set by equations (1) with no nonlinearity) given in the vicinity of the cylinder near two cylinder radii. For other parameter values the initial conditions are taken from the data available for the previous value of the parameter.

2.2. Numerical method

The system of equations (1) is solved numerically using the finite volume method on the Cartesian grid. The domain is discretized on two different meshes: $720 \times 60 \times 240$ and $1440 \times 120 \times 480$ designated as $P$. This allows one to perform comparison in terms of the mesh convergence. The nonlinear inviscid part of the equations is discretized using WENO-5 schemes with modified smoothing indicators, see [9]. The viscous tensor is discretized using the 4-th order central scheme. The temporal discretization is performed using the third order Runge-Kutta method [10]. The method for the inviscid part of the equations was extensively benchmarked in [11]. The viscous part of the equations was benchmarked using synthetic solution approach.

The treatment of boundary conditions is conducted in the characteristic manner with the damping parameters in order to prevent the spread of unphysical perturbations inside the domain. The method for the characteristic boundary conditions is discussed in [12] and is
implemented in the analogous way with the usage of WENO instead of Lagrange interpolation near the boundary.

Numerical implementation is done on the computational architecture based on the multiple Graphics Processing Units (GPUs) communicated between each other by the means of the Message Passing Interface (MPI) with direct GPU-PCI-bus communications. In this study we used three and five NVIDIA k40 GPUs.

3. Methods of analysis

The main method of analysis is based on the phase space analysis and Poincaré sections and the application of the Proper Orthogonal Decomposition (POD). The first method is analogous to [13] and [14]. The phase subspace of a smaller dimension is projected from phase space of the dimension 5N by considering a specific points in the physical domain where the vector of conservative variables $U(Q) = (\rho, \rho u_1, \rho u_2, \rho u_3, \rho E)^T$ is evaluated and stored for each temporal step. In this study the set of projecting points in $\Omega$ is defined as:

$$Q = \left\{ \{0.5, 0.5, 3.0\}, \{5.0, 0.5, 3.0\}, \{10.0, 0.5, 3.0\}, \{10.0, 0.5, 1.0\}, \{10.0, 0.5, 5.0\}, \{14.0, 0.5, 3.0\}, \{16.0, 0.2, 3.0\} \right\}.$$ 

In order to construct multidimensional Poincaré sections we take data form different points of the set $U(Q)$ and use slices with the given gap thickness $\delta = 1 \cdot 10^{-5}$.

In order to analyze the flow behavior from the modal viewpoint one uses the POD method [15]. The coherent structures are extracted from the flow and the flow is decomposed into a minimal number of basis functions or modes to capture as much energy as possible. Here the method of snapshots is used [16], since the size $5P$ is beyond any computer to handle the full eigenproblem. For further reading we recommend the review paper [17].

In order to perform the POD analysis one must operate on the fluctuating data that is obtained as $Y(t, \xi) = U(t, \xi) - \langle U(t, \xi) \rangle_{T,R}(\xi)$ for a given value of the parameter value $R$ and averaging time $T$, where $\xi \in \Omega$ is a set of discrete points that represent the spatial discretization of the problem. The averaging operator has property that $\| < Y(t, \xi) >_{T,R}(\xi) \| \leq \varepsilon$ and is called Reynolds averaging, thus the spatial and temporal scales are separated. Theoretically, $\varepsilon = 0$, but in numerical calculations one sets a small predefined value. In this study we used $\varepsilon = 1.0 \cdot 10^{-4}$. Once the averaging is obtained, one can view the expansion of the flow field as:

$$Y(t, \xi) = \sum_{j=1}^{M} a_j(t) \psi_j(\xi),$$

where the vectors $\psi_j(\xi)$ are the expansion functions and

$$a_j(t) = \langle Y(t, \xi), \psi_j(\xi) \rangle,$$  \hspace{1cm} (6)

are the expansion coefficients and $(\cdot, \cdot)$ is the inner product. The space $M = \text{span}\{\psi_j\}_{j=1}^{M}$ is the finite dimensional subspace that exactly expands the sought functions $Y(t, \xi)$ if $M = N$.

The aim of the dimension reduction problem is to reduce the dimension of $M$ and find a value of $m$ in such a way that:

$$Y(t, \xi) = \sum_{j=1}^{m} a_j \psi_j(\xi) + \sum_{j=m+1}^{M} a_j \psi_j(\xi),$$

and

$$\sum_{j=1}^{m} |a_j| / \sum_{j=1}^{M} |a_j| \leq 1. \hspace{1cm} (7)$$
In this case one captures "most" of the dynamics by considering only first \( m \)-basis vectors in the expansion. For the discrete set of points for the temporal steps \( t \in [0, ..., T] \) the POD method attempts to minimize the value of \( m \) by finding the vectors \( \{ \psi : (\psi_j, \psi_k) = \delta_{j,k}, \forall j = 1, ..., m; k = 1, ..., m \} \) (called the POD modes) by solving the following problem:

\[
\sum_{t=0}^{T} \left\| x(t, \xi) - \sum_{j=1}^{m} a_j(t) \psi_j(\xi) \right\|_2^2 \to \min_{\{\psi_j\}_{j=1}^{m}}, \tag{8}
\]

hence the obtained POD modes are optimal from the energy (kinetic energy) point of view.

In other words one can consider the problem (8) as the problem of finding such submanifold \( \mathbb{M} \) that is fitted into an inertial manifold of the original problem (assuming the original problem has one) in the least squares sense. Hence the POD modes \( a_j \) can be considered as the temporal evolution of the reduced dynamical system that is obtained from the original large problem. In this study we shall apply the first method of the analysis to the phase subspace that is generated by the reduced dynamical system and compare the attractors of the system to the original one.

The method of snapshots constructs the POD in the following manner. Let \( N = qP \), where \( q \) designates the number of variables in the conservative vector, in this case \( q = 5 \) and \( P \) is the size of the discrete problem. Suppose that the discrete set \( \{ \tau \} \) of timesteps is available with \( |\{ \tau \}| = M, M << N \). For each element \( t_k \in \{ \tau \} \) we have a vector \( Y(t_k) \in \mathbb{R}^N \) that is obtained from the numerical simulation of the problem. The matrix \( X \in \mathbb{R}^{N \times M} \) can be formed by stacking the vectors as columns of the matrix \( X \). It is assumed that the most significant flow details are represented in the chosen timesteps. Following the method of snapshots, we can form the matrix \( X^TX \in \mathbb{R}^{M \times M} \). One can find the eigenvalues and eigenvectors of the obtained matrix by solving the eigenvalue problem:

\[
X^TX \varphi_j = \lambda_j \varphi_j, \forall j = 1, ..., M. \tag{9}
\]

The obtained eigenvalues are real non-negative numbers since the matrix \( X^TX \) is symmetric positive semi-definite. The original POD method is working with the matrix \( XX^T \in \mathbb{R}^{N \times N} \), i.e. one solves the eigenproblem \( XX^T \psi_k = \theta_k \psi_k, \forall k = 1, ..., N \). However the non-zero eigenvalues of these matrices coincide. The eigenvectors for the original POD matrix are the orthonormal POD modes \( \psi_j \) and are obtained from (9) as:

\[
\psi_j = \lambda_j^{-1/2} X \varphi_j,
\]

for any \( j \in [1, ..., M] \).

The dimension of the reduced system \( m \) can be found by comparing the cumulative sum of the obtained eigenvalues in the same manner as in (7), i.e. the value of \( m \) is chosen such that:

\[
r = \left( \sum_{j=1}^{m} \lambda_j \right) \left( \sum_{j=1}^{M} \lambda_j \right)^{-1} \lesssim 1. \tag{10}
\]

A particular value of \( m \) is chosen by setting the threshold value to \( r \). This value depends on the problem parameter \( R \) and is evaluated for different values separately. The phase space that is generated by the reduced POD modes after the value of \( m \) is selected can be monitored through the expansion coefficients (6).
4. Results and discussion

Let us introduce the designations that are used in our previous papers [18, 19] do indicate bifurcation schemes. A bifurcation scheme is a relation of the form:

\[ p(q_1) \rightarrow p(q_2, q_3) \rightarrow \ldots \rightarrow p(q_i, q_m) \rightarrow \ldots \]

where \( p(q_j) \) indicates the bifurcation type or classification of the phase portrait \( p \) (up to a homeomorphism) for the bifurcation parameter value \( q_j \) or values \( q_k, q_l \), such that the phase portrait \( p \) is valid for \( [q_k, q_l] \). We use the following designations: \( P \) is a stable point, \( sn \) is a saddle-node bifurcation, \( h \) is a supercritical Hopf-Andronov bifurcation, \( Cn \) is a limit cycle of period \( n \), \( nTm \) is an invariant torus of dimension \( n \) formed by limit cycle of period \( m \) and \( Ch \) is a chaotic solution.

We shall call the flow turbulent when the solution is \( Ch \).

The following transition to turbulence is observed:

\[ P_1(0.0, 4.0) \rightarrow sn(4.0) \rightarrow P_2(4.0, 55.0) \rightarrow h(55.0) \rightarrow C1(55.0, 98.0) \rightarrow \]
\[ \rightarrow h(98.0) \rightarrow 2T1(98.0, 103.0) \rightarrow h(103.0) \rightarrow 3T1(103.0, 108.0) \rightarrow Ch, \]

which can be represented in the physical space by isosurfaces of density in figure 1 for parameter values from 45 to 200. The transition (11) represents a classical supercritical transition process to chaotic solutions.

The first three bifurcations are classical results of the linear stability theory and benchmark data, see [1, 20, 21]. The first bifurcation is the transition from the pure creeping flow to the advection dominated regime and, in terms of dynamical systems, presented by the transcritical bifurcation at \( R = 4 \). The corresponding flow regime is presented in figure 1 for \( R = 45 \). Observe, that the first Hopf-Andronov bifurcation at \( R = 55.0 \) is delayed compared to the one from the data [20], which is known to be around 46. The parameter value at the bifurcation point is verified for different considered grid resolutions and \( R = 55.0 \) is stable with maximum error of 3%. This is, most likely, due to the different boundary conditions on the \( z = 0 \) and \( z = 6 \) planes and substantial value of the Mach number at which one can no longer assume the flow to be incompressible. The resulting attracting set is a limit cycle, the physical space that represents the limit cycle regime is presented in figure 1 for \( R = 60 \) and its phase subspace projections in the control points \( Q_j \) are presented in figures 3, 4, 5, and 6. One can observe a preserved symmetry of the flow w.r.t. the \( z \)-velocity component. The flow stays uniform along the \( y \) direction and basically looses stability in the same manner as a 2D flow would in total compliance with the Squire’s theorem. The decay of POD eigenvalues is presented in figures 2 left. One can observe that the POD decomposition for the stable periodic orbit is well converged. The cumulative sum in figure 2 right, gives us the value \( m = 5 \) with \( r = 0.998721 \). Hence the dynamical system with attracting set of dimension one is represented by 5 POD modes almost exactly.

The second Hopf (sometimes called Neimar-K-Sacker) bifurcation at \( R = 98 \) is responsible for the formation of the two-dimensional invariant torus in the phase space. The phase subspace projections in the control points \( Q_j \) are presented in figures 9, 10, 11, and 12. The corresponding physical space is presented in figure 1 for \( R = 105 \). By considering the phase space projections one can observe the symmetry preservation in the \( z \)-velocity component. The POD eigenvalues decay slower with \( m = 30 \) for \( r = 0.998123 \), figure 2. If one applies the criterion \( r = 0.955 \) that was used in [22] for the analysis of 2D flow over the cylinder, then one obtains \( m = 7 \). The reduced phase space of POD modes for \( m = 8 \) also contains an invariant torus that is presented in figure 8. An invariant torus can be observed in the Poincare section that is shown in red in these figures. In order to analyze the capabilities of the possible order reduction in POD, we saved the set of POD mode vectors for \( m = 15 \) and \( k = \{u_x, u_y, u_z\} \), designated as \( \{\psi^k_{100,j}\}_{j=0}^{m-1} \).
and apply those modes for the snapshot flow data for the greater value of the parameter. Some representatives of these POD vectors are shown in figure 17. This, to some extent, will simulate the reduced order system dynamics and will allow us to compare the attracting set generated by the original and POD-reduced dynamical systems.

The third Hopf bifurcation is observed at $R = 103$. The resulting attracting set is a three-dimensional invariant torus. The phase subspace projections at points $Q_j$ and appropriate first and second Poincare sections are presented in figures 13, 14 for $R = 105$. On the left column of the phase subspace projections one can observe the embedded first Poincare sections in different coordinates. A 2D torus in the first section is visible in coordinates $\{u_x := u, u_z := w, E\}$. One can observe that the second Poincare section represents a closed curve. The symmetry in the velocity $z$-component is preserved, see figure 13 right.

The POD eigenvalues at $R = 105$ decay slightly slower than those at $R = 100$ and $m = 46$ for $r = 0.998929$ and $m = 8$ for $r = 0.955$, see figure 2. The phase spaces generated by the POD modes with $m = 15$ are presented in figures 15 where one can trace the same 3D invariant torus (requires more data to generate second Poincare sections). The application of the POD modes for $R = 100$ with the data from $R = 105$ results in the chaotic solution, see figures 16. The reduced order model, obtained from $\{\psi_{100, j}^k\}_{m=0}^{m-1}$ is not applicable for $R = 105$ and the reduced dynamical system is poorly approximated by the selected POD modes.

Another bifurcation is observed at $R = 108$ which generates a chaotic solution. At this point no regular structures can be observed in the phase subspace projections. It is highly likely that some form of crisis is formed at that parameter value. The POD decomposition at $R = 115$ has a slow decay of eigenvalues, see figure 2. For the cumulative sum value $r = 0.99875$ one obtains $m = 145$ and for $r = 0.955$ one obtains $m = 21$. The symmetry in the $y$-direction is lost and the flow exhibits a substantially 3D structure, see figure 1 for $R = 200$. Further search is underway to understand the transition process at higher values of the Reynolds numbers. No period doubling bifurcation is observed. It means that there exist more than one scenario of transition to turbulence depending on the problem formulation and one cannot postulate a universal scenario even on the initial stage of the transition.

5. Conclusion

- Bifurcation scheme is obtained that shows the classical supercritical transition to chaos.
- The obtained scheme indicated the transition through the cascade of invariant tori. This confirms the results in [3] and extends them to the compressible subsonic flows.
- The POD mode analysis is performed. It is shown that for the same amount of energy in the commutative sum ($r \approx 0.998$) the number of active modes suffers quadratic grows rate, at least, with the increase of the Reynolds number.
- The POD reduced model doesn’t produce a correct attracting set of the dynamical system for the extrapolation. The reduced order models can’t predict precise low dimensional dynamics in the range of the parameter extrapolation.

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Figure 1. Instantaneous isosurfaces of density for different Reynolds numbers in the process of transition to turbulence.
Figure 2. Decay of the first 600 POD eigenvalues, left, cumulative sum of the first 25 eigenvalues [10], right.

Figure 3. Phase subspace projections at $Q_1$ for $R = 60$, periodic orbit.

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Figure 5. Phase subspace projections at $Q_3, Q_6$ for $R = 60$, periodic orbit.

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Figure 6. Phase subspace projections at $Q_4, Q_5$ for $R = 60$, periodic orbit.

Figure 7. Phase subspace projections of POD modes for $u_j = a_{x,j}$ and $w_j = a_{z,j}$ for $R = 60$, periodic orbit.

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Figure 8. Phase subspace projections with embedded Poincare section (red) of POD modes for $u_j = a_{x,j}$ and $w_j = a_{z,j}$ for $R = 100$, 2D invariant torus.

Figure 9. Phase subspace projections with embedded Poincare section at $Q_1$ for $R = 100$, 2D invariant torus.
Figure 10. Phase subspace projections with embedded Poincare section at $Q_2$ for $R = 100$, 2D invariant torus.

Figure 11. Phase subspace projections with embedded Poincare section at $Q_4$ for $R = 100$, 2D invariant torus.
Figure 12. Phase subspace projections with embedded Poincare section at $Q_5$ for $R = 100$, 2D invariant torus.
Figure 13. Phase subspace projections with embedded first Poincare section at $Q_2$ for $R = 105$ at different coordinates (left column), first Poincare section and second Poincare slice ($u_2 = 0.6$) of the 3D invariant torus (right column).
Figure 14. Phase subspace projections with embedded first Poincare section at $Q_4$ for $R = 105$ at different coordinates (left column), first Poincare section and second Poincare slice ($u_4 = 1.15$) of the 3D invariant torus (right column).
Figure 15. Phase subspace projections with embedded Poincare section (red) of POD modes (top row), Poincare sections (bottom row) for $u_j = a_{x,j}$ and $w_j = a_{z,j}$ for $R = 105$, 3D invariant torus.
Figure 16. Phase subspace projections with embedded Poincare section (red) of POD modes (top row), Poincare sections (bottom row) for $u_j = a_{x,j}$ and $w_j = a_{z,j}$ for $R = 105$, using POD modes $\{\psi_{100,j}\}_{j=0}^{14}$. 
Figure 17. Four POD modes for $u_z := w$ velocity component at $R = 100$ multiplied by $\sqrt{\lambda_j}$. 