Supplemental Material:
Dynamics-based machine learning of transitions in Couette flow

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1 Data availability
All trajectories we use in this Letter are generated with the open-source computational fluid dynamics library Channelflow [1]. The velocity field \( u(x, t) \) is stored in discrete spatial locations \( u(x_j, y_j, z_j, t) \) due to the spectral discretization. A sample of the generated data is available under the link [2]. In addition to the raw data, we also made available the codes used for the analysis in the form of a commented MATLAB® live script, as a part of the open-source toolbox SSMLearn [3]. The full data set is available from the authors upon request.

2 Spectral Submanifolds
In this section, we briefly recall the properties of spectral submanifolds (SSMs) in general dynamical systems.

Based on the two periodic directions (along \( x \) and \( z \)), we discretize the incompressible Navier–Stokes equations [1] by Galerkin-projection onto a Fourier-Chebyshev basis,

\[
\mathbf{u}(x, y, z, t) = \sum_{k_z, k_x, n_y} \mathbf{u}_{k_z, k_x, n_y}(t) T_{n_y}(y) e^{2\pi i (k_x x/L_x + k_z z/L_z)},
\]

where \( T_m(y) \) is the \( m \)-th Chebyshev polynomial. The sums in (1) are taken over a finite number of wave-numbers denoted by \( k_z, k_x \) and Chebyshev-modes indexed by \( n_y \). With this discretization, the time-evolution of the spectral coefficients is governed by the following ordinary differential equation

\[
\frac{d}{dt} \hat{\mathbf{u}} = A \hat{\mathbf{u}} + \mathbf{f}(\hat{\mathbf{u}}), \quad \mathbf{f}(\hat{\mathbf{u}}) \in O(||\hat{\mathbf{u}}||^2),
\]

where we have introduced the single vector \( \hat{\mathbf{u}} \in \mathbb{R}^N \) to be collection of all spectral coefficients of all three velocity components. The matrix \( A \in \mathbb{R}^{N \times N} \) represents the linear part of the dynamics, and all nonlinear terms are collected in \( \mathbf{f}(\hat{\mathbf{u}}) \), which is a \( C^\infty \) smooth function. The matrix \( A \) and the coefficients of \( \mathbf{f} \) can be obtained by substituting (1) in the Navier–Stokes equations and enforcing incompressibility to eliminate the pressure \( p \).

Equation (2) describes a finite-dimensional dynamical system, to which the results of [4] are applicable. Those results do extend to infinite dimensions [5] but require technical assumptions that would be challenging to verify for the Navier-Stokes equations [6].

Let us assume that \( \mathbf{u}_0 \) is a hyperbolic fixed point of (2). In our case, this could represent the laminar base state, the lower- or upper branch Nagata invariant solutions. Because of the hyperbolicity of the fixed points representing these states in the phase space, the local dynamics around \( \mathbf{u} \) is determined by the linear part, which is the matrix \( A \). We define a spectral subspace as the vector space spanned by a set of eigenvectors of \( A \). Any such subspace is invariant under the linearized dynamics. Important special cases of spectral subspaces are the stable and unstable subspace, which are spanned by the eigenvectors of \( A \), whose eigenvalues have strictly negative and strictly positive real parts, respectively. By the center manifold theorem [7], the nonlinear system (2) has corresponding invariant
manifolds (called stable and unstable manifolds) that are tangent to the unstable and stable subspaces at the fixed point.

As discussed in [4, 5], such stable and unstable manifolds are further foliated by lower-dimensional invariant submanifolds that are tangent to spectral subspaces of the unstable and stable subspaces. We focus here on the slowest spectral subspaces spanned by the eigenvectors associated to the eigenvalues with decay rates closest to zero. We denote by \(E_d\) such a \(d\)-dimensional spectral subspace, where \(d = 1, 2\) will hold in the present paper. A spectral submanifold (SSM) will then be a \(d\)-dimensional invariant manifold, \(W_d\) of the full nonlinear system that is tangent to \(E_d\) at the fixed point \(\hat{u}_0\). There is an abundance of such invariant manifolds already in the linearized system, so the non-uniqueness of \(W_d\) in the nonlinear system is fully expected. Nevertheless, building on prior work by [5], the theorems of [4] establish the existence of a unique smoothest \(W_d\) under appropriate non-resonance conditions on the spectrum \(\text{Spect}A\) of \(A\).

To state these results, we first define the spectral quotient corresponding to the spectral subspaces \(E_d\) as

\[
\sigma(E_d) = \text{Int} \left[ \max_{\lambda \in \text{Spect}A} |\text{Re} \lambda|, \min_{\lambda \in \text{Spect}A_{E_d}} |\text{Re} \lambda| \right],
\]

where \(\text{Spect}A_{E_d} = \{\lambda_1, ..., \lambda_d\}\) denotes the restriction of the spectrum of \(A\) to the spectral subspace \(E_d\). In our present setting, (2) arises from the discretization of the Navier–Stokes equations, and hence its linear part has eigenvalues with arbitrarily large negative real parts [8], making \(\sigma(E_d)\) infinite. In practice, \(\sigma(E_d)\) is a large positive number of the order of a 100, whose exact value depends on the level of the discretization used in obtaining eq. (2).

We call the spectral subspace \(E_d\) non-resonant if

\[
\sum_{i=1}^{d} m_i \lambda_i \neq \lambda_j, \quad \lambda_j \in \text{Spect}A - \{\lambda_1, ..., \lambda_d\}
\]

hold for any set of nonnegative integers \(m_i \in \mathbb{N}\) satisfying \(2 \leq \sum_{i=1}^{d} m_i \leq \sigma(E_d)\). We note that the non-resonance conditions stated here are generically satisfied, i.e., hold with probability 1. Even if the spectrum of the underlying PDE were resonant due to symmetries, these would not be exact resonances in the finite-dimensional truncation [5].

The main result of SSM theory is that for any nonresonant \(E_d\), a (primary) SSM defined above exists that is unique among all \(C^{\sigma(E_d)+1}\) invariant manifolds tangent to \(E_d\) at the fixed point \(\hat{u}_0\). All other invariant manifolds (secondary SSMs) tangent to \(E_d\) at \(\hat{u}_0\) are only \(C^r\) smooth with \(r < \sigma(E_d) + 1\).

We note that although the finite-dimensional representation of the Navier–Stokes was formulated in terms of the spectral coefficients, the SSMs can also be found in the phase space of velocity measurements. By Whitney’s embedding theorem [9], the SSMs will be smoothly embedded in the high-dimensional space of the velocity measurements with probability 1.

3 Parametrizing spectral submanifolds with the rate of energy input and the dissipation

From simulations we note a one-to-one correspondence between the dynamics on the SSMs and that of \(I\) and \((I, D)\), for the one- and two-dimensional SSMs respectively. Hence, we can use these variables to parametrize the SSMs for the full velocity field. In the main text, we choose \(J = \sqrt{|I|}\) and \(K = \sqrt{|D|}\) instead of \(I\) and \(D\).

To motivate our choice, we consider the case in which the SSM is one-dimensional, but similar considerations hold for the other regimes investigated in this Letter. Figure 1 shows the dependence of the flow field on the coordinates \(I\) and \(J\). We display the streamwise velocity (the \(u\) component) in 4 spatial locations in the channel. The inset in the lower right of Fig. 1 shows a power-law type behavior of \(|u(x_j, 0, z_j)|/(I)|\) with exponent 1/2.
Note that in the left panel of Fig. 1, the trajectory has a vertical tangent at the origin, and hence the velocity components near \( I = 0 \) cannot be expressed as a smooth graph over \( I \). Due to this singularity, the derivative with respect to \( I \) diverges. The right panel shows that viewing the flow field as a function over \( J \) resolves this issue as the graph no longer has a vertical tangent at \( I = J = 0 \). Therefore, the vector-valued coefficients \( \mathbf{w} \) in the parametrizations of the SSM can be expressed as

\[
\mathbf{u}(x, y, z, t) = \mathbf{u}_{\text{base}} + \sum_{l+m=0}^{M_p} \mathbf{w}_{l,m}(x, y, z) J^l(t) (\text{Re} - \text{Re}_c)^m \quad \text{in region (I)},
\]

\[
\mathbf{u}(x, y, z, t) = \mathbf{u}_{\text{base}} + \sum_{l+m \leq M_p} \mathbf{w}_{l,m}(x, y, z) J^l(t) K^m(t) \quad \text{in regions (II) and (III)},
\]

where we have parametric dependence in \( \text{Re} \), measured from a reference value \( \text{Re}_c \), for regime (I).

To identify the coefficients of the parametrization, we minimize the \( L^2 \) norm of the difference between the velocity field \( \mathbf{u} \) and its reconstruction. That is, the coefficients are obtained by minimizing the error

\[
\mathbf{w}^*_{l,m} = \arg \min_{\mathbf{w}_{l,m}} \sum_{j=1}^{N_{dp}} \left\| \mathbf{u}(x, y, z, t_j) - \mathbf{u}_{\text{base}} - \sum_{q+r=0}^{M_p} \mathbf{w}_{q,r}(x, y, z) J^q(t_j) (\text{Re} - \text{Re}_c)^r \right\|_{L^2}^2 ,
\]

for the \( N_{dp} \) data-snapshots available, whose solution is that of a least-squares minimization problem [10].

### 4 Additional details of the reduced dynamical models

We use reduced dynamics of the form

\[
J_{n+1} = R(J_n, \text{Re}) \quad \text{in region (I)},
\]

\[
\begin{pmatrix}
J_{n+1} \\
K_{n+1}
\end{pmatrix} = \begin{pmatrix}
R_1(J_n, K_n) \\
R_2(J_n, K_n)
\end{pmatrix} \quad \text{in region (II)}.
\]

Figure 1: Dependence of the streamwise velocity \( u \) on the energy input \( I \) and on its square root \( J \), measured at 4 points in the channel. The trajectory is initialized on the unstable manifold of the lower-branch and converges to the base state, at \( \text{Re} = 134.52 \). The inset in the lower right shows the absolute values of the velocity measurements as a function of \( I \) on logarithmic scales.
In region (I), we allow for Reynolds-number-dependent coefficients in the polynomial expansion of the function $R$ up to first order. We look for $R$ in the form

$$R(J, \text{Re}) = \sum_{l=1}^{M_2} \sum_{m=0}^{1} R_{l,m} \partial^l (\text{Re} - \text{Re}_c)^m,$$

where $\text{Re}_c = 134.5$ is a reference value for the Reynolds number, around which we take the expansion. In the two-dimensional regime (II), the reduced dynamics is

$$R_{1,2}(J, K) = \sum_{l,m: l+m \leq M_4} R_{l,m}^{(1,2)} J^m K^l.$$

In all cases, we denoted the maximal order in the polynomial expansions by $M_4$. The coefficients of the reduced dynamics are obtained from data by SSMLearn, and, for cases (I) and (II), the a priori knowledge of non-trivial fixed points is given to the model identification. Specifically, the discrete time dynamical system $\eta_{n+1} = r(\eta_n, \mu)$ on the state variable $\eta \in \mathbb{R}^m$ depending on the parameters $\mu \in \mathbb{R}^d$ and with $N_{fp}$ fixed points can be identified from $N_{dp}$ data points by solving the constrained minimization problem

$$r^* = \arg \min_r \sum_{j=1}^{N_{dp} - 1} \|\eta_{j+1} - r(\eta_j, \mu_j)\|^2 + \sum_{l=1}^{N_{fp}} 2\lambda_l \|r(\eta_{fp,l}, \mu_{fp,l}) - \eta_{fp,l}\| + C_p(r),$$

where $\lambda_l$ for $l = 1, 2, ..., N_{fp}$, are the Lagrange multipliers and $C_p(r)$ is a regularization term. For the polynomial representations of $r$ in Eqs. (5) and (6) and a ridge-type penalty, their coefficients are identified by solving problem (7) in closed form. Specifically, this representation takes the form $r(\eta, \mu) = \eta + R\varphi(\eta, \mu)$ where the feature map $\varphi$ denotes the selected $N_m$ multivariate monomials in $(\eta, \mu)$ and $R \in \mathbb{R}^{m \times N_m}$ is a matrix containing their coefficients. As we center around the base (laminar) state, we need to assume that $0 = r(0, \mu)$, which implies that the monomials have at least linear dependence on the coordinates $\eta$. By indicating the $k$-th component of a vector $\eta$ as $\eta^{(k)}$, we define

$$R^T = \begin{bmatrix} r_1 & r_2 & \ldots & r_m \end{bmatrix}, \quad X^T = \begin{bmatrix} \varphi(\eta_1, \mu_1) & \varphi(\eta_2, \mu_2) & \ldots & \varphi(\eta_{N_{dp} - 1}, \mu_{N_{dp} - 1}) \end{bmatrix},$$

$$y_k = \begin{bmatrix} \eta_1^{(k)} - \eta_1 \ 
 \eta_2^{(k)} - \eta_2 \ 
 \ldots \ 
 \eta_{N_{dp}}^{(k)} - \eta_{N_{dp}} \end{bmatrix}, \quad Y = \begin{bmatrix} y_1 \ y_2 \ \ldots \ y_m \end{bmatrix},$$

$$X_{fp}^T = \begin{bmatrix} \varphi(\eta_{fp,1}, \mu_{fp,1}) & \varphi(\eta_{fp,2}, \mu_{fp,2}) & \ldots & \varphi(\eta_{fp,N_{fp}}, \mu_{fp,N_{fp}}) \end{bmatrix},$$

$$\lambda_k = \begin{bmatrix} \lambda_1^{(k)} & \lambda_2^{(k)} & \ldots & \lambda_{N_{dp} - 1}^{(k)} \end{bmatrix}, \quad \Lambda = \begin{bmatrix} \lambda_1 \ \lambda_2 \ \ldots \ \lambda_m \end{bmatrix},$$

and let $L \in \mathbb{R}_{N_m \times N_m}$ a diagonal matrix whose values are the maximum absolute values taken along the columns of $X \in \mathbb{R}^{N_{dp} \times N_m}$. Then, we can reformulate problem (7) using the cost function

$$C(R, \Lambda; \lambda) = \sum_{k=1}^{m} \|y_k - Xr_k\|^2 + \langle \lambda_k, X_{fp} r_k \rangle + \lambda \|Lr_k\|^2,$$

as $(R^*, \Lambda^*) = \arg \min C(R, \Lambda; \lambda)$, whose solution is

$$
\begin{bmatrix} R^{*-T} \\ \Lambda^* \end{bmatrix} = \begin{bmatrix} X^TX + \lambda L^2 & X_{fp}^T \\ X_{fp} & 0 \end{bmatrix}^{-1} \begin{bmatrix} X^TY \\ 0 \end{bmatrix},
$$

where the parameter $\lambda$ is determined via cross-validation [10]. We remark that analogous developments hold for the case of a vector field $\dot{\eta} = r(\eta, \mu) = R\varphi(\eta, \mu)$, in which one would only need to set $y_k$ in (9) as a vector of time derivatives. Table 3 summarizes the maximal polynomial orders for the parametrization $M_f$ and for the reduced dynamics $M_d$ with which the results in the main text were obtained.

Figure 2 shows the mapping $R(J, \text{Re})$. In the left panel, we show its value over the $(J, \text{Re})$ plane. For training, we use a total of 6 trajectories, which are initialized on the unstable manifold of the lower-branch fixed point for 3 different Reynolds numbers, Re = 134.51, 134.52, 134.53. The right panel show the curve of fixed points satisfying $J = R(J, \text{Re})$, obtained by continuation on the reduced model, that reproduces the saddle-node bifurcation of the
Table 1: Maximal polynomial orders used in the expressions of the reduced dynamics ($M_d$) and in the parametrization of the SSM ($M_p$).

|       | Region (I) | Region (II) | Region (III) |
|-------|------------|-------------|--------------|
| $M_d$ | 15         | 4           | 5            |
| $M_p$ | 6          | 2           | 5            |

full model. For numerical continuation, we use the MATLAB® open source continuation core software coco [11]. In Fig. 3, the mapping of the reduced dynamics in region (II) is plotted. For simplicity, we only plot one of the components, $R_1$, in the plane $(J, K)$.

Figure 2: Left panel: the mapping $J_{n+1} = R(J_n, \text{Re})$ on the one-dimensional SSM with the three curves of fixed points are shown. Right panel: lower- and upper-branch fixed points in the $(I, \text{Re})$ plane obtained by numerical continuation. The blue curve shows the stable branch and the unstable branch is plotted in yellow. Colored circles indicate the Reynolds numbers at which training trajectories were initialized.

Figure 3: The mapping $J_{n+1} = R_1(J_n, K_n)$ on the two-dimensional SSM. Colored circles indicate the three fixed points.
4.1 Region (III)

In region (III), we find that a reduced-order model based on a two-dimensional manifold containing all transitions cannot be constructed. This is because the unstable manifold of the lower branch spirals onto a limit cycle, and hence is not a differentiable manifold. To infer the minimal dimension of a higher-dimensional SSM containing the transition, we show in Table 4.1 the leading eigenvalues of all coexisting ECSs at Re=146.

Table 2: The leading four eigenvalues of the coexisting ECSs at Re=146. The eigenvalues are in descending order based on their real parts (decay rate). In the last column, the Floquet exponents of the limit cycle are reported. These are defined as $\lambda = \frac{1}{T} \log \Lambda$, where $\Lambda$ is the Floquet multiplier and $T$ is the period of the limit cycle.

Based on the spectrum of the limit cycle, the slowest smooth SSM that captures the lower transition orbit would be four-dimensional.

Instead of a higher dimensional model, in region (III), we restrict our analysis to a neighborhood of the limit cycle, which allows us to represent the reduced dynamics via the polar normal form

$$
\dot{\rho} = \sum_{n=0}^{\text{Int} \left( \frac{M_d-1}{2} \right)} c_n \rho^{2n+1}, \quad \dot{\theta} = \sum_{n=0}^{\text{Int} \left( \frac{M_d-1}{2} \right)} d_n \rho^{2n},
$$

(11)

with the variables $(\rho, \theta)$ linked to $(J, K)$ via a nonlinear change of coordinates. The model in Eq. (11) is able to capture the transition from an unstable fixed point to an attracting limit cycle, and its form is reminiscent of the Hopf normal form at first sight. Note, however, that in the classic Hopf normal form, the coefficient $c_0$ is a small bifurcation parameter, whereas in our setting, $c_0$ is not small and no closeness to a bifurcation is assumed. Indeed, we do not perform the classic normal form procedure familiar from center-manifold reduction near non-hyperbolic
fixed points. Instead, we use the data-driven extended normal form methodology outlined in [3] for hyperbolic fixed points, which we briefly review here for our particular setting.

After centering coordinates at the upper state, we first estimate the linear part $\mathbf{R}_1 \in \mathbb{R}^{2 \times 2}$ via regression for the dynamics in the coordinates $(J, K)$. In region (III), the eigenvalues of $\mathbf{R}_1 = \mathbf{PDP}^{-1}$, which are the entries of the diagonal matrix $\mathbf{D}$, are the complex conjugate pair with positive real part $c_0 \pm i\delta_0$, cf. Table 2. As this equilibrium is hyperbolic with nonresonant eigenvalues, the normal form on the SSM would be purely linear [7]. However, the domain of validity of such a linear normal form would be limited and could not capture the transition to a limit cycle. To this end, via the extended normal form procedure of [3], we allow for nonlinear terms (i.e., those with $n > 0$ in Eq. (11)) that would arise in the reduced dynamics if the real part of the eigenvalues of the linearized spectrum on the SSM were zero at the fixed point. This enlarges the domain of validity of our data-driven reduced-order model that is now capable of capturing nonlinear behavior. For our particular case, we set $\mathbf{y} = \mathbf{P}^{-1}(J, K)$ and $\mathbf{z} = (z, \bar{z})$ with $z = r e^{i\theta}$, and we define the set $S(M_d) := \{ (l, m) \in \mathbb{N}^2 : 2 \leq l + m \leq M_d, l \neq m + 1 \}$ to be used in the near-identity change of coordinates

$$y = z + h(z) = (h_1(z, \bar{z}), \bar{h}_1(z, \bar{z})), \quad h_1(z, \bar{z}) = z + \sum_{(l, m) \in S(M_d)} h_{l,m} z^l \bar{z}^m. \quad (12)$$

The inverse transformation, $\mathbf{z} = h^{-1}(\mathbf{y})$ features the same monomial structure. The dynamics takes the complex normal form of that in [11], i.e.,

$$\dot{z} = n(z) = (n_1(z, \bar{z}), \bar{n}_1(z, \bar{z})), \quad n_1(z, \bar{z}) = \sum_{n=0}^{\text{Int} (M_d-1)/2} (c_n + i\delta_n) z^{n+1} \bar{z}^n. \quad (13)$$

Note that the nonlinear monomials present in the normal form do not appear in the coordinate changes $h_1, h_1^{-1}$. We then find the nonlinear coefficients of the mappings $h^{-1}$ and $n$ via minimization of the conjugacy error

$$\left(h^{-1*}, n^* \right) = \arg \min_{h^{-1}, n} \sum_{j=1}^{N_{dp}} \left\| \frac{d}{dt} h^{-1}(y_j) - n \left((h^{-1}(y_j)\right) \right\|^2, \quad (14)$$

for the $N_{dp}$ trajectory datapoints available. The nonlinear coefficients of $h$ are estimated via regression afterwards, when the coordinates $\mathbf{z}$ are known. This extended normal form identification problem is solved automatically by the SSMLearn algorithm.

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