Course project for "Statistical mechanics II: Chaos and what to do about it (2001)"
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Chaotic laminar shear dispersion in a swirling flow.

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Abstract: Although laminar shear dispersion mechanisms are known to mix passive scalars at rates that are orders of magnitude higher than by molecular diffusion, it is even higher if the velocity field causes chaotic particle trajectories. The objective here is to lay the groundwork to calculate global averages like lyapunov exponents, diffusion rates, transport coefficients etc. for a given steady laminar flow field with chaotic particle trajectories, by using the tools developed in periodic orbit theory (POT) of hyperbolic dynamical systems. The given flow field is a steady three-dimensional swirling flow in a closed cylinder with a rotating bottom boundary condition. This velocity field is a solution to the 3d Navier-Stokes equation for a Reynolds number of 1400. At this *Re* the velocity field is steady and has already bifurcated to form a single steady breakdown bubble. A poincare map is calculated for the $\theta = 0$ plane in cylindrical polar coordinates and periodic prime-cycles up to period 20 identified using a multipoint newton-rapshon search algorithm. All the period-one orbits are centers with complex eigenvalue while most orbits with higher time periods are saddles. Stability and time periods of these periodic orbits are used to evaluate various cycle expansion formulas of POT.

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1. **Introduction**

Passive scalars in any fluid flow mix due to two fundamental processes namely, molecular diffusion and dispersion. Out of these, diffusion is understood as a deterministic process happening due to the collision of molecules causing exchange of momentum and positions. Often in fluid flows this process is much slower than mixing due to dispersion (often called stirring). Dispersion is said to have taken place if any scalar blob present in the flow is stretched and folded by the transporting velocity field thereby causing the blob to occupy an ever-growing amount of space of the flow field with time. In the case of bounded flows, the scalar blob eventually occupies all the available space and asymptotically approaches a uniform scalar concentration over the entire space.

Any transporting velocity field of flows in nature is always three dimensional and non-linear. Therefore it is very likely that the fluid elements within such flows have chaotic trajectories. Even in the simplest case where the flow field is steady, one may still expect chaotic trajectories due to the non-linear nature of the field. Living among such flows, how does one study the dispersion of scalar blobs in them? Such a study is very important from an engineering point of view where reactors, mixers, diffusers etc. are the objects of design in many industries such as chemical, mechanical, civil and environmental etc. Flow fields in these objects are typically turbulent and therefore constitute the frontiers of such studies. The most simplest flow fields however are laminar and steady. Even such flows may be of potential interest to objects of nano-technology where one may build a reactor whose size does not allow for turbulent mixing. Study of dispersion in such simple flows will be a good groundwork to study turbulent dispersion.

This article sums up the study of a particular steady laminar flow that has attracted appreciable amount of attention in literature due to its simple, yet rich dynamics. The flow is in a cylinder with a rotating bottom boundary condition. The Reynolds number of the flow is 1480 and is a steady laminar velocity field. This flow also belongs to the class of swirling flows due to the driving Ekman layer at the rotating boundary. Treating the cylinder as a mixer, the objective is to calculate the mixing properties of this flow field using the tools developed in periodic orbit theory of finite dimensional chaotic dynamical systems. The analysis involves finding only those fluid elements that return to their original position after a finite time. The trajectory of such a particle is a periodic orbit and the set of all such periodic orbits constitutes a dense subset of the cylinder. In other words the closure of this set is the entire phase space (here the set of all positions occupied by the fluid). A direct result of the periodic orbit theory is that any long-term description of a finite dimensional chaotic dynamical system is purely a function of the set of periodic orbits along with their stabilities alone. Therefore properties, depending on long-term behavior, such as global averages, transport coefficients, diffusion rates, entropies and Lyapunov exponents etc. are a function of the dense set of periodic orbits. By calculating the stabilities of these periodic orbits, one can extract the exact values of the long-term properties by summing over all the periodic orbits, in the so called cycle expansion formulas. These infinite sums are convergent for most types of chaotic systems and calculation of periodic orbits up to a short time period is sufficient to obtain a reasonable estimate to their exact values. Such an analysis of a given flow field is presented in the following sections.

2. Background

The dynamical system studied is given by the following equations

$$\begin{aligned} \dot{x} &= U(x, y, z) \\ \dot{y} &= V(x, y, z) \\ \dot{z} &= W(x, y, z) \end{aligned} \qquad (1)$$

Where *u*, *v* and *w* are the velocity field satisfying the Navier-Stokes equations for the rotating lid container problem. The flow field is in a cylinder of radius *R* and height *H* filled with an incompressible Newtonian fluid of kinematic viscosity ν. Boundary conditions involve one end of the cylinder rotating at a constant angular velocity ω while the rest of the cylinder is held fixed. Non-dimensionalizing the governing equations yields two parameters namely the aspect ratio, H/R, and the Reynolds number $Re = \omega R^2/\nu$. The flow field in (1) corresponds to an aspect ratio of 2.0 and $Re = 1480$. The solution to the Navier-Stokes equation is that obtained by Sotiropoulos & Ventikos (2001) who solved numerically the unsteady, three-dimensional Navier-Stokes equations using a second-order-accurate finite-volume method. The solution is obtained on a curvilinear mesh with 150x97x97 grid nodes in the axial and transverse direction. To obtain the velocity at a point within a computational cell, the tri-linear interpolation is used as follows:

$$\vec{U}(x,y,z) = \vec{A}_1 xyz + \vec{A}_2 xy + \vec{A}_3 xz + \vec{A}_4 yz + \vec{A}_5 x + \vec{A}_6 y + \vec{A}_7 z + \vec{A}_8 \qquad (2)$$

where the coefficients A_i are calculated by solving an 8x8 linear system of equations for every cell.

3. Dynamics

Integration of equation (1) yields the trajectories of fluid particles advected by the velocity field. The calculated typical trajectories within the cylinder are shown in Figure 1. From the figure it is clear that particles at the bottom of the cylinder are accelerated away from the cylinder axis due to the rotation and therefore spiral their way upwards and then dive back to the bottom close to the axis at the top of the cylinder. The flow also has a vortex breakdown bubble at the center, which may have resulted from a bifurcation due to instabilities in the flow. The breakdown bubble is better visualized by calculating trajectories only using the *U* and *W* components of the velocity field. Figure 2 shows the visualization of the bubble and also some qualitative trends in the flow.

From the periodic orbit theory, all the long-term behavior of (1) is governed solely by the set of periodic trajectories alone. Inorder to find these periodic trajectories, a poincare map is calculated for the $\theta = 0$ plane (*XY* plane with $X>0$, $Y>0$). Inorder to generate the map, a grid of 300x1000 particles are placed on the XY plane respectively and the image of each particle on the same plane is calculated by integrating each initial point until each trajectory intersects with the plane. A bi-linear interpolation is used to find the image of any particle within a cell as follows:

$$\begin{aligned} X_{n+1} &= B_1 X_n Y_n + B_2 X_n + B_3 Y_n + B_4 \\ Y_{n+1} &= C_1 X_n Y_n + C_2 X_n + C_3 Y_n + C_4 \end{aligned} \qquad (3)$$

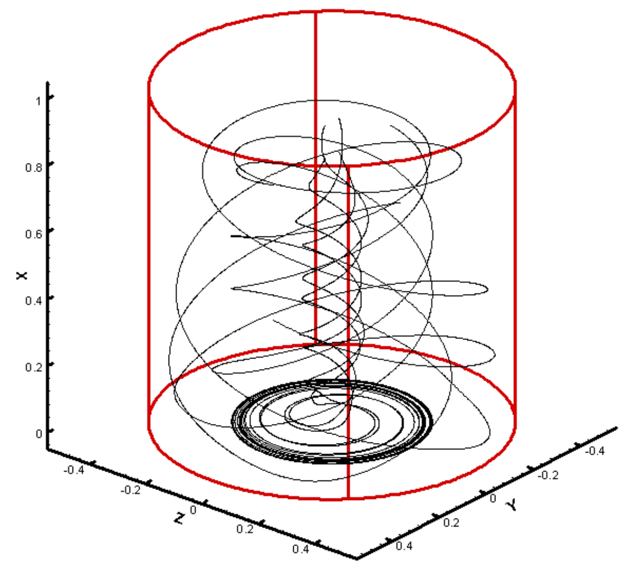

Figure 1. Typical trajectories inside the cylinder (*X* is axial direction, *Y* and *Z* are transverse direction)

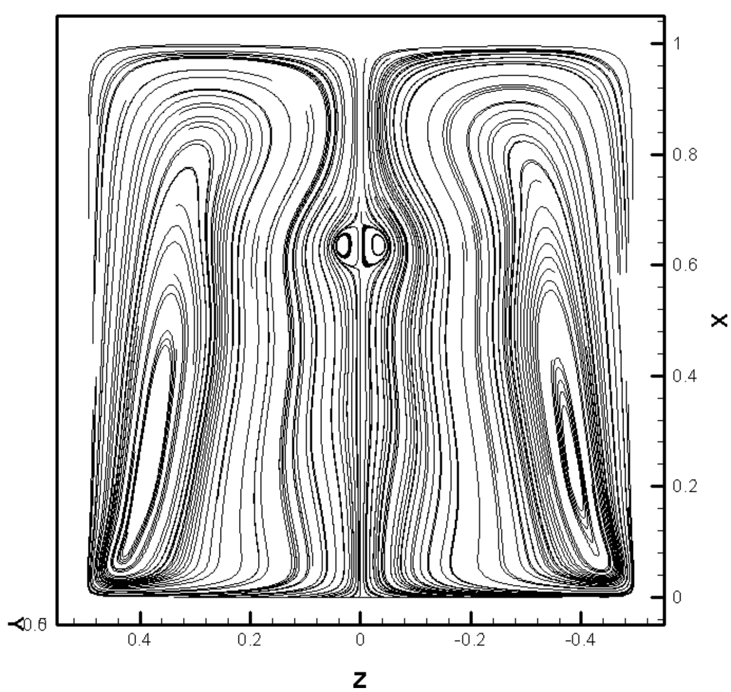

Figure 2. Visualization of the breakdown bubble located on the axis of the cylinder.

Figure 3 shows the first iterates of an initial 300x1000 grid of particles placed on the $\theta = 0$ plane. From the figure it is clear that although the flow in the cylinder is incompressible, a poincare map appears nowhere close to a Hamiltonian map. However, the neighborhood of any periodic cycle must be mapped in an area preserving fashion (determinant of the Jacobian equals unity). Now, since the set of all periodic cycle points is a dense subset of the map's phase space, one can expect the determinant of the map to equal unity on a dense subset of the map.

Locating the periodic orbits in the poincare map is done using a multi-point shooting Newton-Rapshon algorithm. Figure 4 shows periodic prime-cycle points up to period 10. The eigenvalues of the Jacobian of the nth iterate of the poincare map are also calculated.

4. Periodic orbit theory

Given a chaotic system, the periodic orbit theory enables the exact calculation of observables depending on the long-term behavior of the system. Such observables included averages, transport coefficients, lyapunov exponents, diffusion rates etc. For any observable $a(\mathbf{x})$, a scalar valued function of the phase space . The expectation value $<a>$ can be defined as a space time average in the phase space of the dynamics as follows:

$$< a >= \lim_{t\to\infty} \frac{1}{|M|} \int_M dx \frac{1}{t} \int_0^t d\tau a(x(\tau)) \qquad (4)$$

Inorder to obtain $<a>$ it makes more sense to first examine the evolution of a scalar funtion by the Perron Frobenius operator as:

$$< \exp(\beta A^t) >= \frac{1}{|M|} \int_M dx \int_M dy \delta(y - f^t(x)) \exp(\beta A^t(x)) \qquad (5)$$

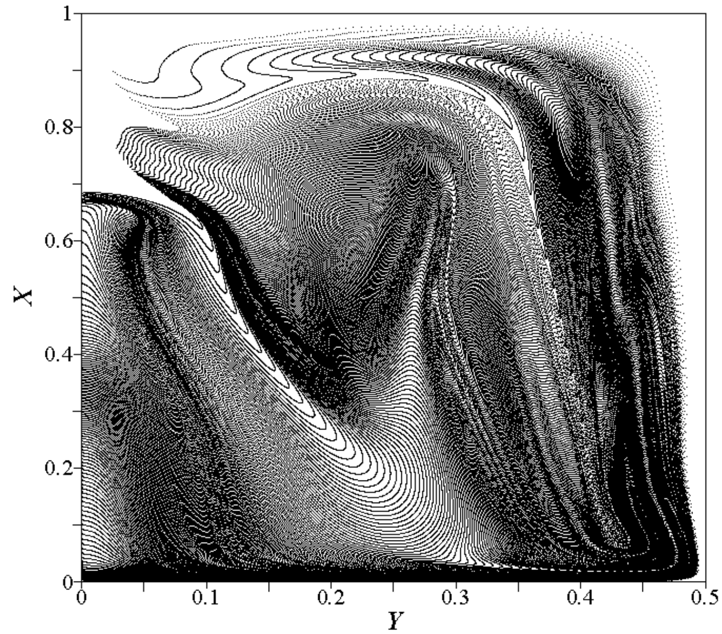

Figure 3. First iterate of 300x1000 particles on θ = 0 plane.

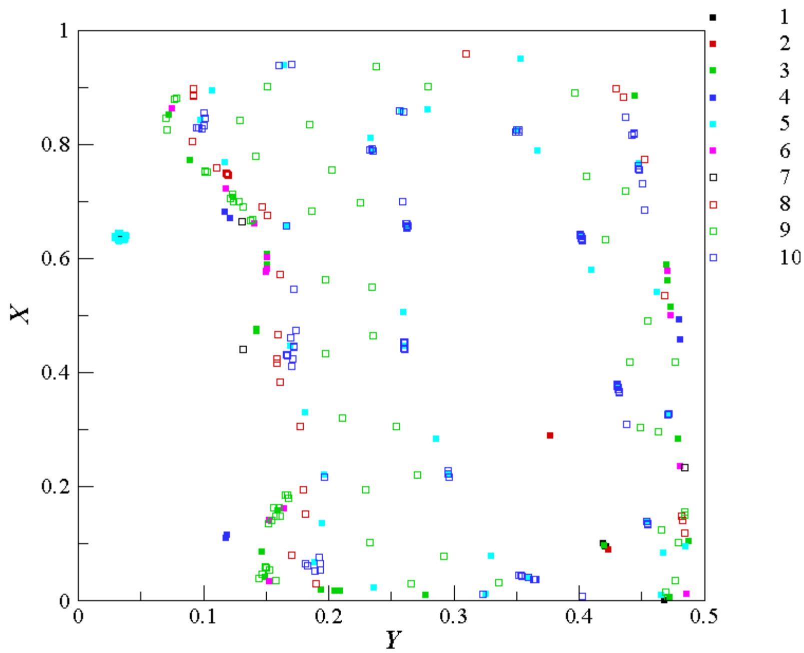

Figure 4. Prime cycles in the poincare map corresponding to a periodic trajectory

Where $A^t = \int_0^t d\tau a(x(\tau))$ is the cumulative of the observable $a(\mathbf{x})$. As t → ∞ one can expect the integral in (5) to grow exponential as follows

$$< \exp(\beta A^t(x)) > \propto \exp(ts(\beta)) \tag{6}$$

where the growth rate goes to a limit

$$s(\beta) = \lim_{t\to\infty} \frac{1}{t} \ln < \exp(\beta A^t) > \tag{7}$$

It can be easily shown that the derivatives of the above function at β=0 are infact statistical moments of the observable of interest. For example:

$$\left.\frac{\partial s}{\partial \beta}\right|_{\beta=0} = \lim_{t\to\infty} \frac{1}{t} < A^t > \qquad =< a > \tag{8}$$

The function s(β) is essentially the leading eigenvalue of the kernel operator in (5). And can therefore be obtained from either the trace of the operator or the determinant of the operator. The leading eigen value is infact the largest zero of the determinant of the characteristic equation of the operator. It can be shown that the spectral determinant of the characteristic equation of the operator in (5) is:

$$\det = \exp\left(-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{\exp\left(r\left(\beta A_p - sT_p\right)\right)}{\left|\det(1 - J_p^r)\right|} \right) \tag{9}$$

The symbols have their usual meanings. Using the above equation, one can calculate the function $s(\beta)$, by finding the zero of (9) for every β. One can therefore calculate (8) upto arbitrary amounts of accuracy.

5. Dispersion rate

Having found periodic orbits and their stabilities, the calculation of dispesion rate for this flow is straightforward. Dispersion in fluid flow is defined as Taylors (1921) "Diffusion by continuous movements". Suppose a particle moves from x(0) to x(t) after a time t, one can define the average position of a particle starting at x(0) as

$$< x >= \lim_{t\to\infty} \frac{1}{t}\int_0^t u\,d\tau \qquad (10)$$

A direct measure of dispersion, in terms of how far a wantering fluid particle may have traveled from its initial position is given by $\left\langle (x-<x>)^2 \right\rangle$. Lets define the dispersion constant *Ds* analogous to the Einstein's definition of diffusion constant as follows

$$Ds = \lim_{t\to\infty} \frac{1}{2dt}\left\langle (x(t)-<x(0)>)^2 \right\rangle \qquad (11)$$

where *d* is the phase space dimension. In (11) <x(0)> is infact the average phase space position of the sytem and is independent of the initial position as any trajectory explores the entire phase space for long times. This quantity can be calculated by setting the observable of interest as the position itself (i.e. $a(\boldsymbol{x}) = \boldsymbol{x}$). Once <x> is obtained, a new observable namely x-<x> can be defined (i.e. $a(\boldsymbol{x}) = \boldsymbol{x} - <\boldsymbol{x}>$). Therefore the dispersion constant can be shown to be:

$$Ds = \frac{1}{2d}\sum_{1}^{d} \left.\frac{\partial^2 s}{\partial \beta_i^2}\right|_{\beta_i=0} \qquad (12)$$

where s(β) is a funtion generated for the observable x(t) - <x>, where <x> is essentially the center of mass of the phase space obtained using the natural measure as the density function.

6. Conclusion and future directions

The periodic theory proves to be an extremely strong theory to calculate averages that depend on long-term behavior from local properties of a dynamical system.

Having found sufficient number of periodic orbits along with their stabilities, the calculation of the function $s(\beta)$ for appropriately chosen observable, inorder to calculate the Dispersion constant will be generated. The Dispersion constant, lyapunov exponents, etc can be calculated for different Reynolds numbers and Swirls. Higher Reynolds numbers would correspond to periodic velocity fields and therefore will increase the phase space dimension by one every time a new period is introduced.

References

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