Effects of the Chaotic Behavior of a Superposition

of Waves in the Flux Across a Channel

by

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Signature of Author Joint Program in Physical Oceanography Massachusetts Institute of Technology Woods Hole Oceanographic Institution August 11, 1999 Certified by Glenn R. Flierl Professor of Oceanography, Department of Earth, Atmospheric and Planetary Sciences Thesis Supervisor Accepted by..... ~ ;· ······ W. Breckner Owens Chairman, Joint Committee for Physical Oceanography Massachusetts Institute of Technology Woods Hole Oceanographic Institution

EFFECTS OF THE CHAOTIC BEHAVIOR OF A SUPERPOSITION

OF WAVES IN THE FLUX ACROSS A CHANNEL

By

CARLOS H. TREVINO LOZANO

Submitted to the Department of Earth, Atmospheric and Planetary Sciences on August, 1999 in partial fulfillment of the requirements for the Degree of Master of Science in Physical Oceanography

ABSTRACT

Several numerical experiments were carried out to study the effects of chaotic behavior on the net tracer flux across a channel. The flow is given by a superposition of two propagating waves. The domain was set up so that a mode-1 wave would fit on it, and the perturbation was a mode-4 wave. The experiments were carried out using a grid model with a second-order upwind differencing scheme. Simple Newtonian diffusion was used, and the velocities were calculated from a streamfunction satisfying no normal flow boundary conditions.

The experiments showed a small increase in the flux does appear due to the chaotic behavior, but this effect is only around 5% when the flux is compared to the one obtained from a pure 1-mode wave system. In contrast there is a difference of around 20% when the pure mode-1 wave is compared to the pure mode-4 wave, the first one being more transportive.

The chaotic behavior of the system is described in detail and a Lagrangian experiment was carried out as well to examine the motion of the particles and to explore a different approach to describing the dispersion of a tracer.

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Introduction.

Mixing is probably one of the more complicated and least predictable processes that affect the behavior of the ocean, yet there are still many aspects of mixing that we do not understand. In particular, what is the link between the small scale mixing (e.g., diffusion) and the large scale stirring processes and how much does each of these control the net tranport of a passive scalar? There has been considerable interest recently in "chaotic mixing" induced by relatively smooth velocity fields which, nevertheless, cause rapid intermingling of fluid particles. Understanding the processes and rates of mixing is of fundamental importance in many oceanic situations. There are many things that can be thought of as tracers, from plankton and pollutants, to the physical properties of the water itself such as temperature or density, and all these "tracers" are of great importance for understanding different aspects of the ocean: biological growth, pollution, or the general circulation.

In the following work I tried to answer one very simple question. When working in an Eulerian frame we often ignore the fact that the particles that compose the whole are moving in a chaotic way. Are there any effects of that chaotic behavior on the dispersion of the tracer? There is of course a local mixing that is affected by the chaotic behavior (Pierrehumbert 1991). The system discussed in this work is a channel through which a superposition of waves is travelling. The question is weather the flux across the channel changes as the chaotic behavior evolves.

Motion of the particles.

Consider the flux through a channel having a wavelike behavior described by a linear superposition of two waves with the following streamfunction:

$$\Phi = \sin(x + c_1 t)\sin(y) + \varepsilon \sin[4(x + c_2 t)]\sin(4y)$$

The velocities are given by:

$$u = -\frac{\partial \Phi}{\partial y}; \qquad v = \frac{\partial \Phi}{\partial x}$$

And we'd like to observe the system following the main wave (I will refer to the mode-4 wave as the perturbation, although for large ϵ it is clearly the other way around). We can make a simple change of variable redefining u' = u - c₁, then:

$$\Psi = \Phi + c_1 y = \sin(x + c_1 t)\sin(y) + \varepsilon \sin[4(x + c_2 t)]\sin(4y) + c_1 y$$

For simplicity, I will also redefine $x = x' - c_1 t$.

$$\Psi = \sin(x)\sin(y) + \varepsilon \sin[4(x - c_1t + c_2t)]\sin(4y) + c_1y$$

= $\sin(x)\sin(y) + \varepsilon \sin[4x - 4(c_1 - c_2)t]\sin(4y) + c_1y$

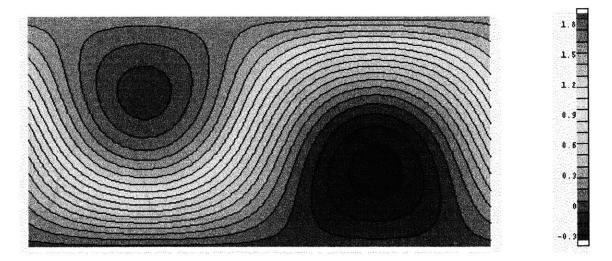
Finally, I will generally use the values $c_1 = \frac{1}{2}$ and $c_2 = \frac{1}{32}$.

$$\Psi = \sin(x)\sin(y) + \varepsilon\sin(4x - \frac{15}{8}t)\sin(4y) + \frac{1}{2}y$$

The behavior resulting from this streamfunction is chaotic (as I will show in brief). When ϵ is very small, or very large the behavior is very simple since it behaves like a single wave (mode-1 or mode-4 respectively). For intermediate values of ϵ (which values exactly is the first question to address) the behavior is very sensitive to the initial conditions. This sensitivity to initial conditions is one aspect of chaos (there are other concepts also referred to as chaos; this system does not for example behave randomly).

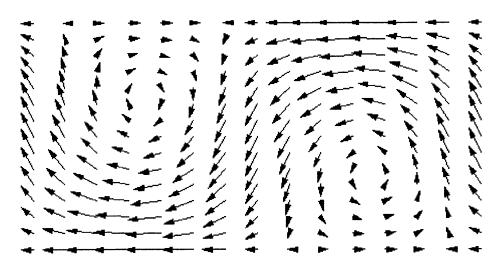
Now suppose we have a source of a certain passive tracer in one side of the channel and a sink on the other. The question I will address in this work is whether or not this chaotic behavior enhances the diffusive transport of the tracer across the channel. Work done by R. T. Pierrehumbert (1990) seems to suggest the chaos produces mixing over large areas quickly spreading a tracer in filaments that are then mixed in the small scale with the surrounding fluid through normal diffusion.

In the following pages I will show in a very informal way how this system behaves and will try to show how this behavior changes for different choices of ϵ . Let's start by looking at the streamfunction and the velocity field when $\epsilon=0$.



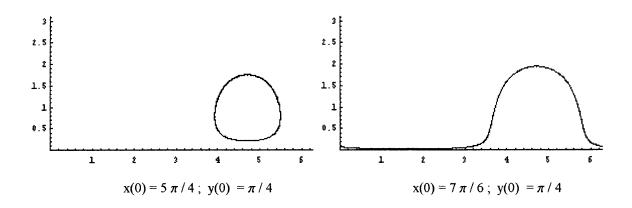
Streamfunction for the unperturbed mode-1 wave.

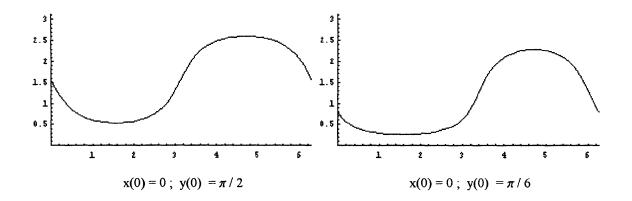
The streamfunction ranges from $-\frac{\sqrt{3}}{2} + \frac{\pi}{6}$ to $\frac{\sqrt{3}}{2} + \frac{\pi}{3}$.



Velocity field for the unperturbed mode-1 wave.

From this second figure we can see there are clearly three different zones with distinct behaviors. There is an area of anti-cyclonic circulation, an area of cyclonic circulation, and a larger area in between with a westward flow. We expect of course that particles into the first two areas will only travel in closed contours (although not necessarily circular), while particles outside these areas will travel following sinusoidal trajectories. At the northern and southern boundaries the meridional velocity is zero, but there is a zonal component. This is just in an infinitely thin layer on the boundary, though, since close to it we have zones of convergence and zones of divergence. For the unperturbed wave the particles move following the shown streaklines so the trajectories are pretty simple. Lets look at some of the trajectories:

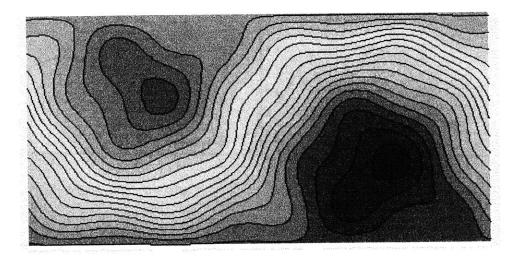




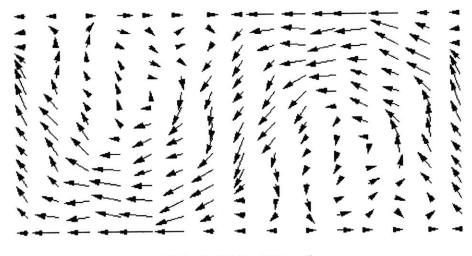
These trajectories have been integrated using Mathematica which in turn uses either a stiff Gear method (orders between 1 and 5) or a non-stiff Adams method (orders between 1 and 12) depending on the requested precision and accuracy, sometimes switching between them.

These trajectories correspond exactly to the streaklines shown in the contour plot of the streamfunction. In that one you can see how the particles go from circular closed orbits, to still closed ellipsoidal-flattened in one side orbits, then abruptly to deformed sinusoidal orbits, and finally to a perfectly symmetric orbit (shown in the third trajectory). In this unperturbed case the particles never depart from these trajectories so the system is clearly not chaotic. This changes however with even the smallest value of ϵ .

We can still examine the streamfunction and the velocity field, although keep in mind the first wave is stationary in our coordinate system but the second wave is not, so these contours are evolving in time. Let's look at some plots for $\epsilon=0.1$.

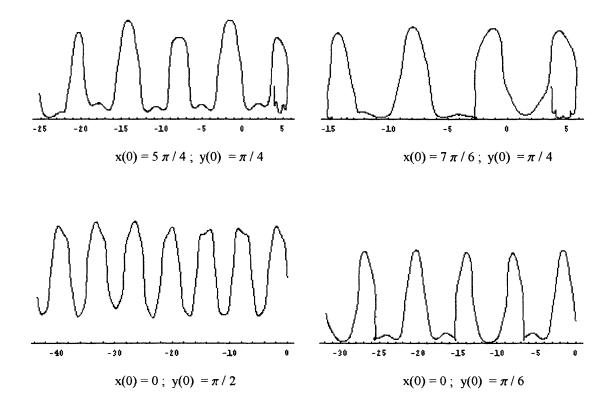


Streamfunction (ϵ =0.1, t=0)

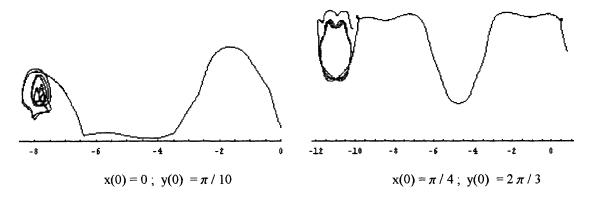


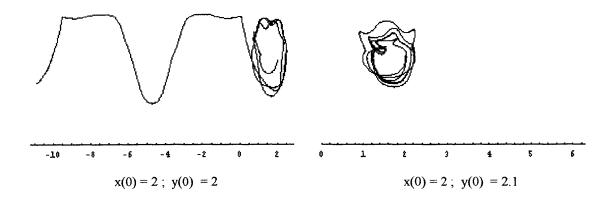
Velocity field (ϵ =0.1, t = 0)

The perturbation does not seem to do much. The streaklines are somewhat deformed, as is of course the velocity field, but just looking at these figures one could think nothing much has changed. In fact the trajectories are now chaotic. Let's revisit the trajectories for the previous starting points (all plotted from time 0 to 50).



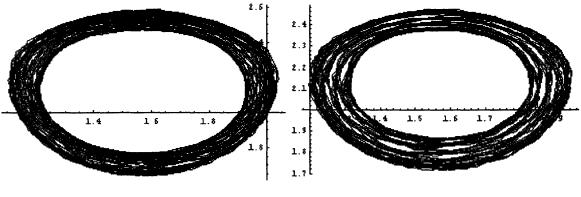
As you can see, the first particle (which was in a closed trajectory) now seems to start describing a closed orbit but quickly falls into an oscillating one. The second one does something very similar although it falls into an orbit with clearly less energy. The third one still does an oscillating orbit although it is clearly deformed around the crests and valleys and the deformation changes from cycle to cycle. The fourth one seems to follow an orbit very similar to the second one, however the zonal displacement has been twice as much. These orbits are perhaps not very illustrative in this case so let's take a look at some more orbits for different starting points.





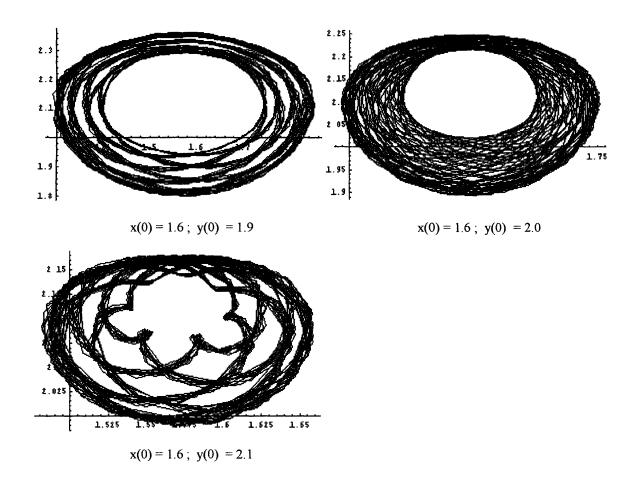
For the first two starting points you can see orbits that start with sinusoidal behavior and then fall into the closed orbit regions. In the third one the opposite happens. In the fourth one although the starting point is just slightly north from the first one (both well inside the closed orbits) the particle didn't leave the same region (at least in this time range). In fact, lets have a closer look at these closed orbits.

Let now ϵ =0.01 (where the chaotic behavior is much weaker). We want to examine how the closed orbits change with slightly different initial conditions. Take a look at the following plots (time range: 0-500).



x(0) = 1.6; y(0) = 1.7

x(0) = 1.6; y(0) = 1.8



These figure show even for a perturbation a hundred times smaller than the main wave the orbits are very sensitive to the initial position.

To really understand the changing behavior of the system with respect to ε we need a more systematic approach. I will do this by using Poincaré maps. However, before going any further I need to talk about the normalization of the streamfunction.

Normalization

When playing with the different parameters of the stream function it is important to keep the energy constant. This can be accomplished by normalizing the function with respect to the energy. This can be done easily integrating the energy (since it's always positive) over the period of the main wave (also the period of the perturbation). If we define the energy as:

$$u^{2} + v^{2} = \cos^{2}(y)\sin^{2}(x) + 8\varepsilon\cos(y)\cos(4y)\sin(y)\sin(4x + (c - c_{2})t) + 16\varepsilon^{2}\cos^{2}(4y)\sin^{2}(4x + (c - c_{2})t) + \cos^{2}(x)\sin^{2}(y) + 8\varepsilon\cos(x)\cos(4x + (c - c_{2})t)\sin(y)\sin(4y) + 16\varepsilon^{2}\cos^{2}(4x + (c - c_{2})t)\sin^{2}(4y)$$

We can then integrate this:

$$\int_{0}^{\pi} \int_{0}^{2\pi} (u^{2} + v^{2}) dx dy = \pi^{2} (1 + 16\varepsilon^{2})$$

and the norm is simply $\pi\sqrt{1+16\varepsilon^2}$

Throughout the rest of this work I will use a constant amplitude of π , so the normalized stream function (in the moving frame) becomes:

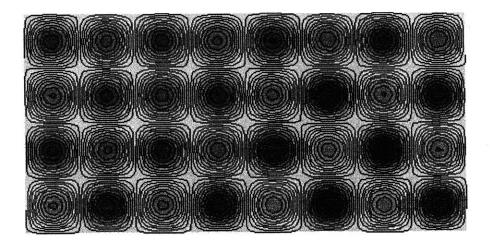
$$\Psi(x, y, t) = \frac{1}{\sqrt{1 + 16\varepsilon^2}} [\sin(x)\sin(y) + \varepsilon \sin(4x + (c - c_2)t)\sin(4y)] + cy$$

The total energy in the system is π^2 for the static frame, or if we calculate the energy in the moving frame it is $\pi^2(1+2c^2)$.

Poincaré maps.

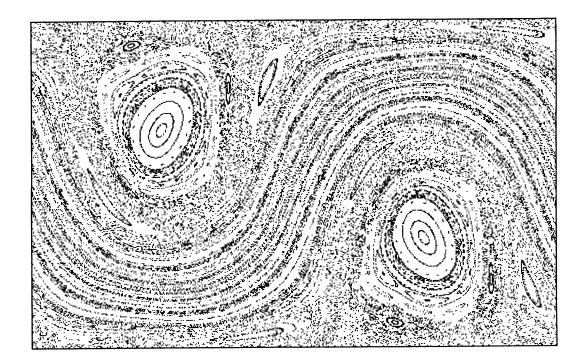
Chaos theory is by now an old subject going back perhaps to the Poincaré solution to the 3-body problem (1889). There are nowadays very sophisticated mathematical tools for analyzing chaotic systems and thousands of papers published in the subject. My purpose however is a simple one, so I will limit myself to the use of Poincaré maps to try to find out how the system behavior changes for different values of ϵ . Pierrehumbert (1990) does a more complete analysis on a very similar problem, especially using Lyapunov exponents and some statistical tools.

In the following pages I show Poincaré maps for several different values of ϵ . These were constructed starting from a grid of 225 points and plotting 200 points for each starting position. Since the first wave is stationary the points were plotted every 16 π / 15, which is the period of the second wave. Keep in mind that for small values of ϵ the main wave is dominant so we expect the particles to follow corresponding trajectories. For big values of ϵ the orbits correspond to a non-stationary mode-4 wave so we should see some circular orbits corresponding to something like the following streamfunction (ϵ =10, t=0).

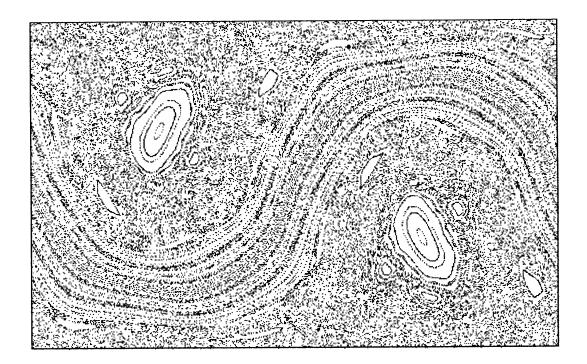


Streamfunction (ε =10, t=0)

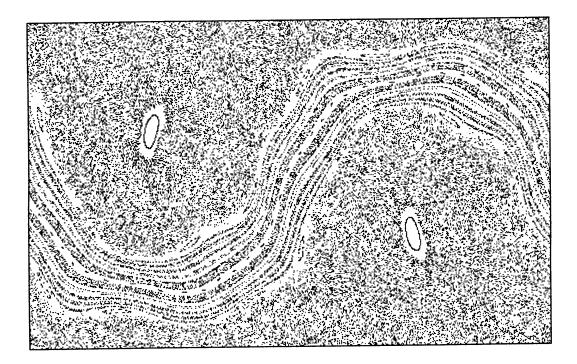
The really interesting behavior is, of course, for values in between, where the system is more chaotic and neither of the waves is really dominant.



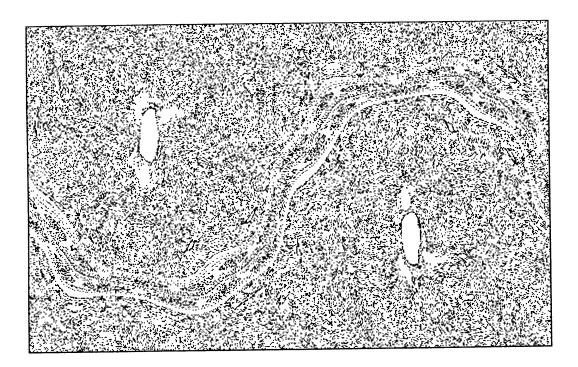
ε = 0.01



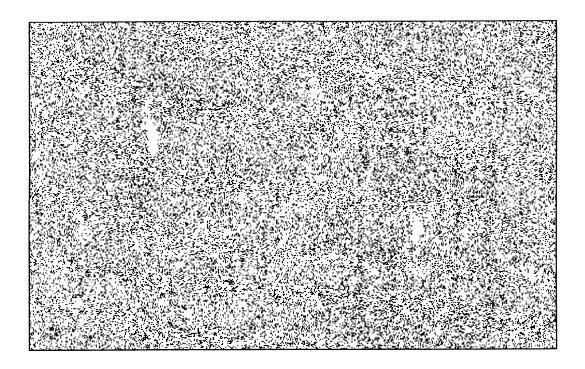
 $\epsilon = 0.025$



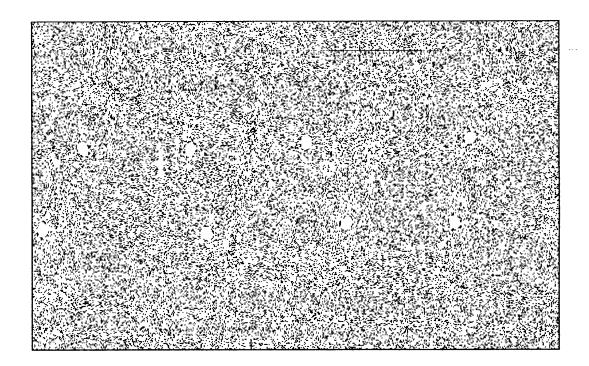
 $\epsilon = 0.05$



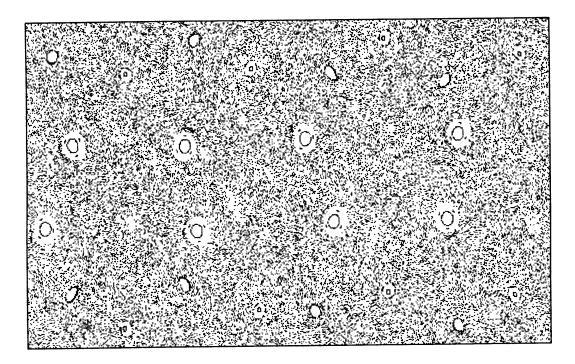
 $\varepsilon = 0.075$



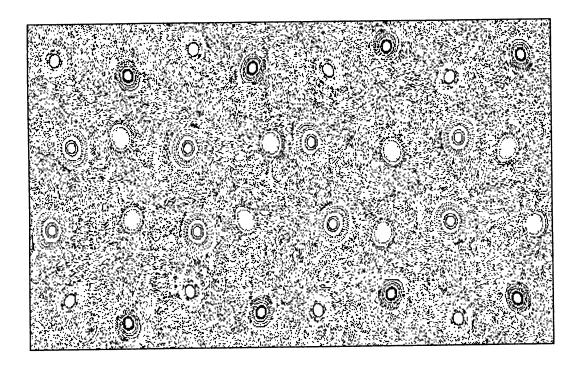
 $\varepsilon = 0.1$



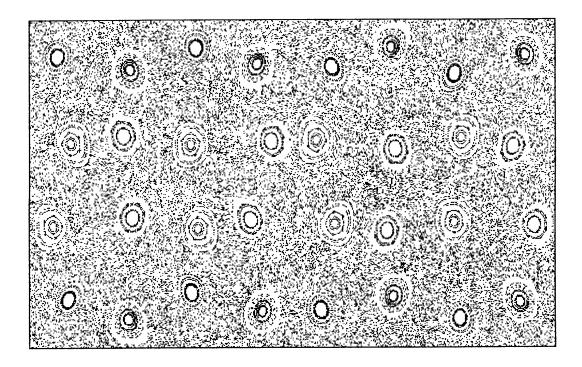
ε = 0.25



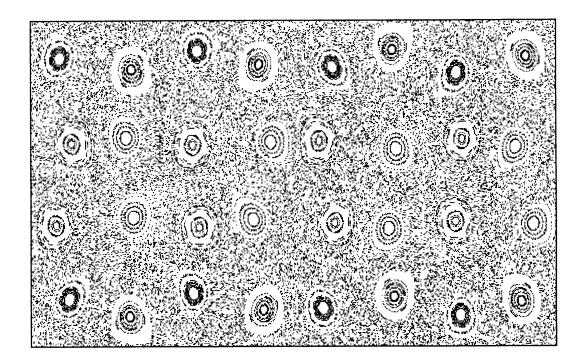
 $\epsilon = 1/3 \ (1/Norm = 0.6)$



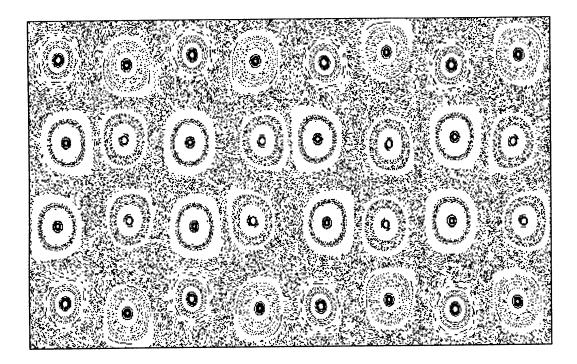
 $\epsilon = \sqrt{3}/4 \ (1/Norm = 0.5)$



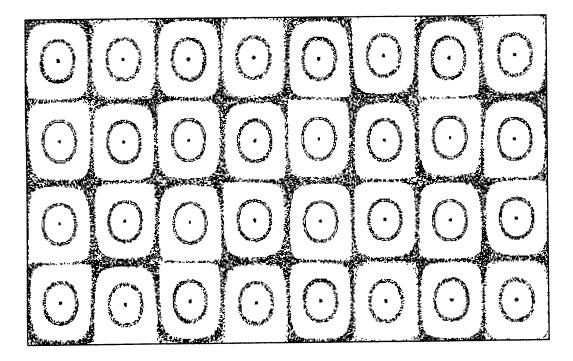
 $\epsilon = 0.5$



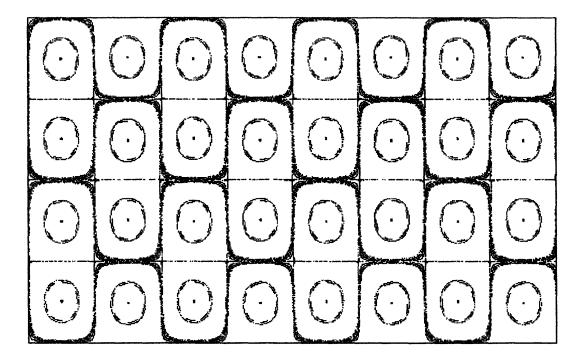
 $\epsilon = \sqrt{21}/8$ (1/Norm = 0.4)



ε = 1

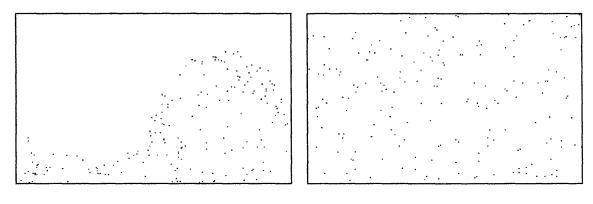


ε = 10





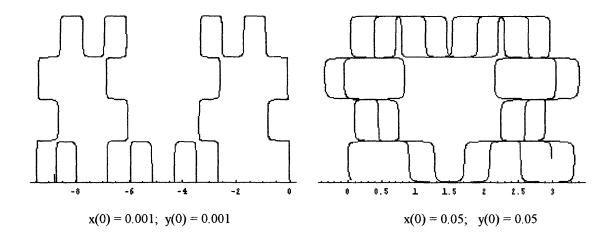
We can learn from these figures several things. For small ε we recognize three distinct zones where the behavior is non-chaotic (the two zones of closed orbits and the sinusoidal orbits in the middle) and two growing zones of chaotic behavior in between. At first these two zones are separated. However on the map for $\varepsilon = 0.1$ the two zones seem to have merged. In fact this is not true yet. Although the sinusoidal orbits have virtually disappeared there is still a separatrix. We can see this clearly is we look at a map constructed with the points corresponding to only one starting point in the southwest corner.



 $\varepsilon = 0.1$

 $\varepsilon = 0.25$

Although the larger maps look very similar, these two show the behavior has shifted at some point and for ε =0.25 the mode-4 wave is starting to dominate the system. This tendency continues for larger and larger values of ε . For ε =10 the chaotic behavior is mostly gone although the particles follow complicated trajectories like the following.



Diffusion Model (Lagrangian Approach).

One concern that arises when considering the effect of chaos in properties of a flow is how to develop a numerical model that can encompass both the properties of the flow (such as the concentration of any given tracer, which we tend to think of from an Eulerian perspective), and the chaotic behavior itself (which is usually approached from a Lagrangian perspective).

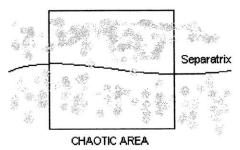
On the one hand we can use a grid model with some diffusion scheme and Eulerian advection. This is a typical approach for modeling something as the flux of a tracer in a flow specified in one way or another. It is not obvious however if the chaotic behavior shown by individual particles within the flow is reflected in the grid model. One obvious scheme one can use to model the Eulerian advection in a grid is to calculate the average velocity on each side of each cell:

$$u_{i,j} = \frac{1}{\Delta y} (\Psi(i\Delta x, (j+1)\Delta y, t) - \Psi(i\Delta x, j\Delta y, t))$$
$$v_{i,j} = \frac{1}{\Delta x} (\Psi((i+1)\Delta x, j\Delta y, t) - \Psi(i\Delta x, j\Delta y, t))$$

Ax

Then one can use this average velocities in many different ways to simulate advection. It is not clear to me, however, if these average velocities actually reflect the chaotic behavior one can see when integrating trajectories for individual particles. Even if it does there are a number of questions that come to mind. What happens if a separatrix runs through the center of a cell, how can the effect of the separatrix be reflected?

CHAOTIC AREA



Another way of approaching this problem is to use a large array of particles, integrate their trajectories and then try somehow to move the properties of the fluid along with the particles. There are also a number of problems with this approach, but I will delay the discussion of those. The following experiment was done using a Lagrangian approach.

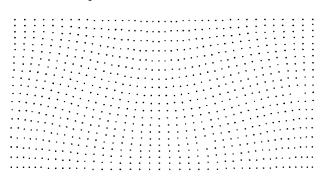
Experiment 1.

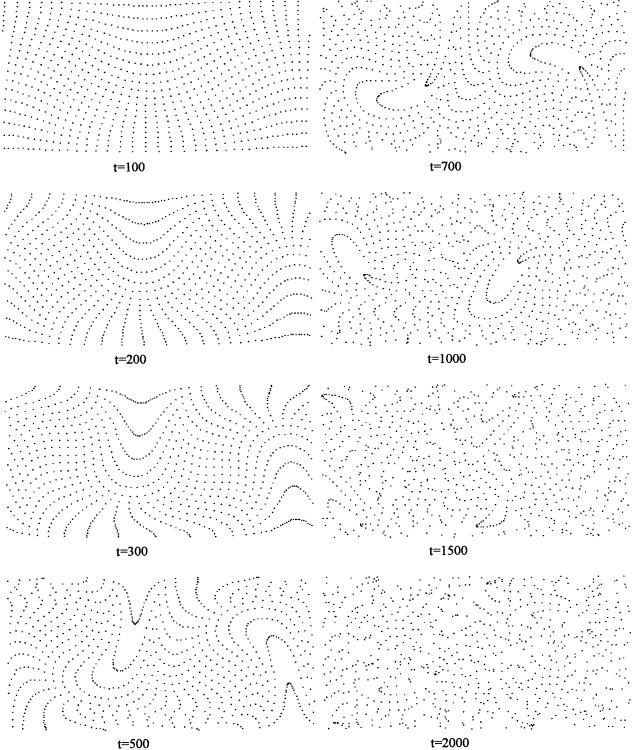
For this first experiment the value of $\varepsilon = 0$. This value corresponds of course to an unperturbed main wave and therefore no chaos at all.

The initial state consisted on a rectangular array of 800 particles. On this array each particle has a tag meant to represent the concentration of the tracer at the position of the particle. On the initial state all the particles had a tag value of zero except for the bottom row which had a value of one.

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Then the trajectory of each particle was integrated over a period of $t = 5\pi$, using the same procedure that was used for the Poincaré maps. This was then mapped to a table with 2000 time steps (from t=0 to t = 5π). The following figures show the position of the particles for different times. The value for the time shown is actually the number of time steps to reach that time.





t=2000

Once the trajectories were integrated and arrays were made with the position of the particles at each time step the next problem was to try to transmit the concentration value tagged to each particle to the surrounding particles. The way this was done was using a Newtonian diffusion scheme to exchange properties between the particles on a one to one basis

$$s_{i}(t_{j+1}) = s_{i}(t_{j}) - \frac{k(t_{j+1} - t_{j})}{\Delta x^{2} + \Delta y^{2}} \sum (s_{i}(t_{j}) - s_{k}(t_{j}))$$

where the summation includes all particles within a radius of length δ . In principle δ could be set to $\delta \rightarrow \infty$ implying that the parcel of fluid where the particle is diffuses onto the entire fluid. Of course distant particles would have little effect since the effect is inversely proportional to the square of the distance. For the purpose of doing this numerically that is indeed an easy approach but very time consuming (computing time). The best thing is to set a finite δ to obtain a minimum Δs .

$$\delta = \sqrt{\frac{k\Delta t}{\Delta s_{MIN}}}$$

For the purpose of this experiment:

k = 0.0025;

$$\Delta t = \frac{\pi}{400};$$

 $\Delta s = 0.0002;$
 $\delta = 0.313329;$

On the other hand there must also be a minimum distance where this scheme holds. If two particles are very close they could easily turn with negative values. The minimum distance allowed is:

$$\lambda = \sqrt{\frac{k\Delta t}{\frac{1}{2}}} = 0.00626657$$

That is, if the particles are a distance λ from each other then $\Delta s=0.5$ (at most, in the extreme case where one particle has s=1 and the other s=0). If the distance is less than λ the particles are simply averaged. If more than one particle is within distance λ all are averaged together.

This solution might seem a little dubious but for this low resolution experiment this is little more than a safeguard. For the given δ an average of around 4 particles were usually within the radius of each particle. That is, we have at least around 1600 interactions (for 800 particles) for each time step. For 2000 steps this adds up to 3.2 million interactions. During the whole experiment not a single interaction had a distance of less than λ . In the next experiment there were only 6 (although only 1200 steps were used).

With δ and λ defined nothing was left but to do the computation. I found the fastest way to iterate through all the particles was to sort the array by coordinates. That way it is possible to iterate for each particle from starting in n+1 (n is the particle index in the sorted array) moving first in the y-direction, then in the xdirection and stopping as soon as $\Delta x > \delta$. This also guarantees two particles will not interact twice.

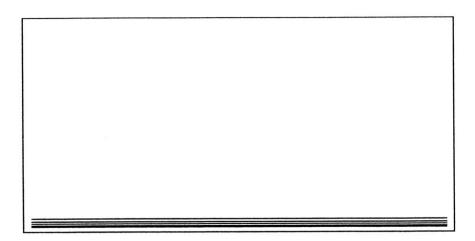
The particles with $x < \delta$ were copied to the end of the array and its interactions mapped to the original particles.

Finally, to visualize the data produced a grid was constructed using the particles, just copying the value of the particle's tag to the cell. The grid was 20x40 so it was to be expected some cells would not have any particles in their area, and some cells would have more than one particle. When several particles were into one cell the tracer concentration in the cell was set to the average of the values of the particles. To fix the cells without any particles on them I used a smoothing algorithm on the x-direction. Basically a value was calculated for the cell using a linear interpolation based on the nearest cells with values.

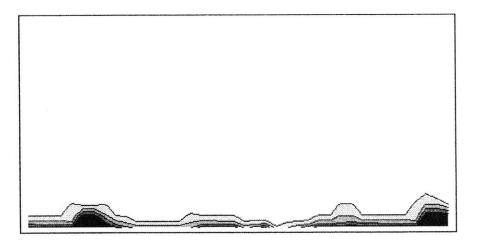
S _i	$\frac{s_i + s_{i+2}}{2}$	<i>s</i> _{i+2}
----------------	---------------------------	-------------------------

S _i	$\frac{2s_i + s_{i+4}}{3}$	$\frac{s_i + s_{i+4}}{2}$	$\frac{s_i + 2s_{i+4}}{3}$	<i>S</i> _{i+4}
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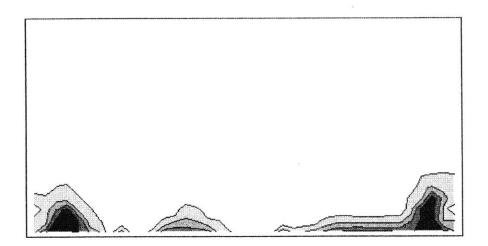
The following pages show the contours produced using this grid for different times.



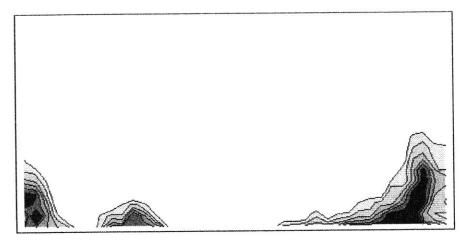
t=0, s=0.9, 0.7, 0.5, 0.3, 0.1



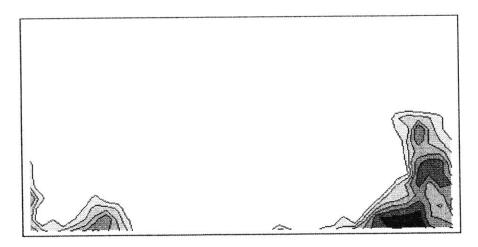
t=100, s=0.7, 0.5, 0.3, 0.1



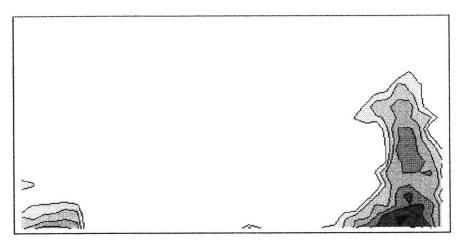
t=200, s=0.7, 0.5, 0.3, 0.1



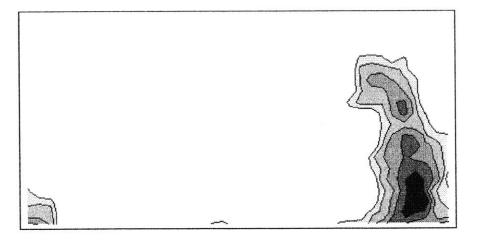
t=300, s=0.6, 0.5, 0.4, 0.3, 0.2, 0.1



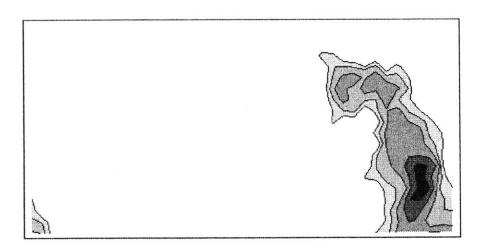
t=400, s=0.6, 0.5, 0.4, 0.3, 0.2, 0.1



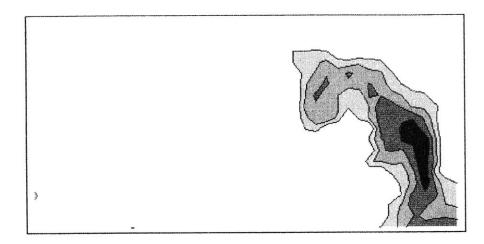
t=500, s=0.6, 0.5, 0.4, 0.3, 0.2, 0.1



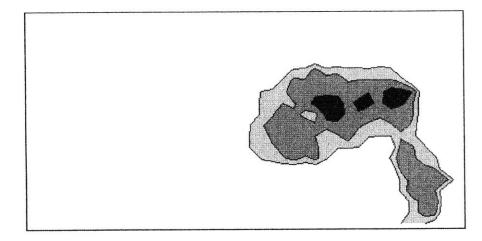
t=600, s=0.5, 0.4, 0.3, 0.2, 0.1



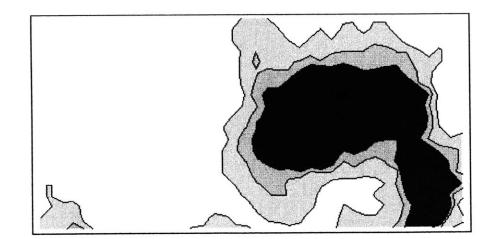
t=700, s=0.5, 0.4, 0.3, 0.2, 0.1



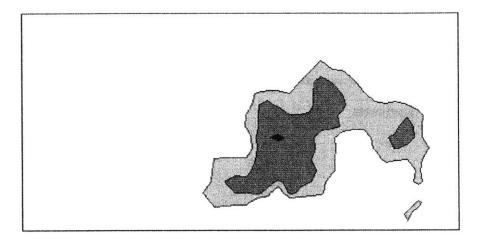
t=800, s=0.4, 0.3, 0.2, 0.1



t=1000, s=0.3, 0.2, 0.1



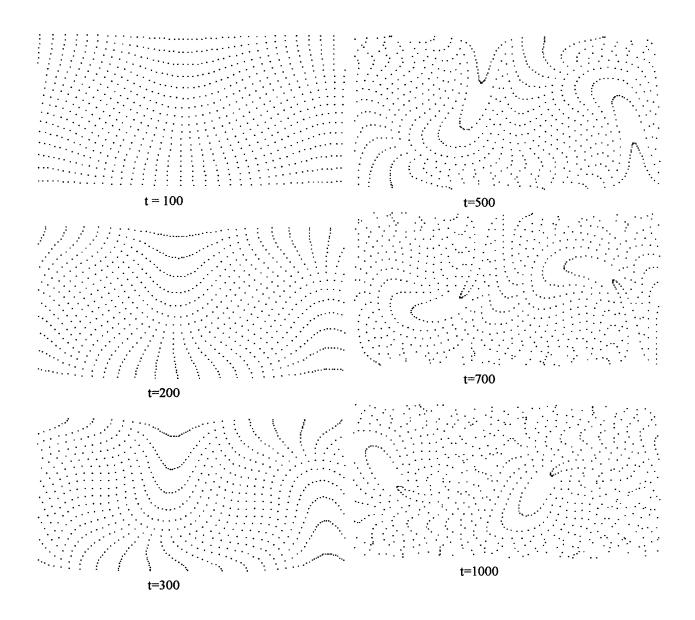
t=1000, s=0.1, 0.05, 0.01

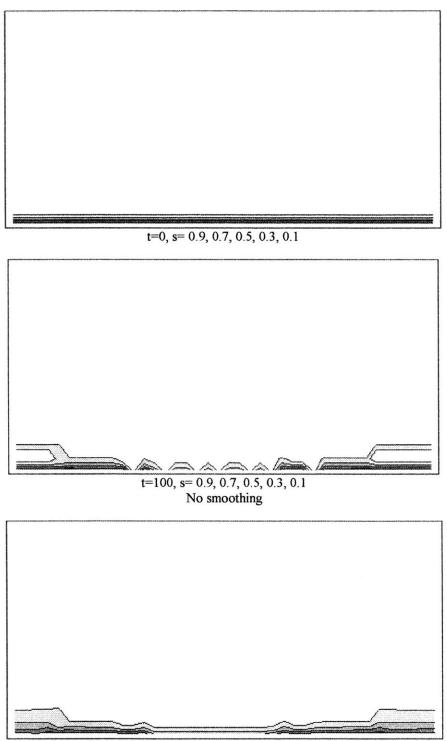


t=1200, s=0.3, 0.2, 0.1

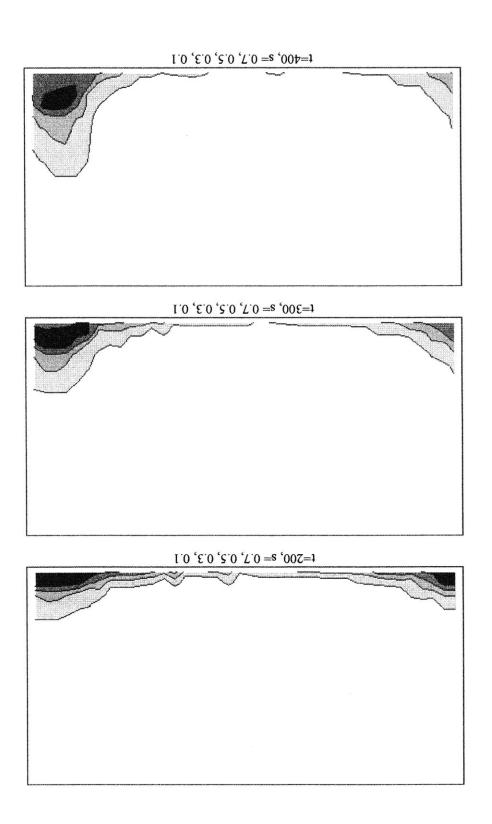
Experiment 2

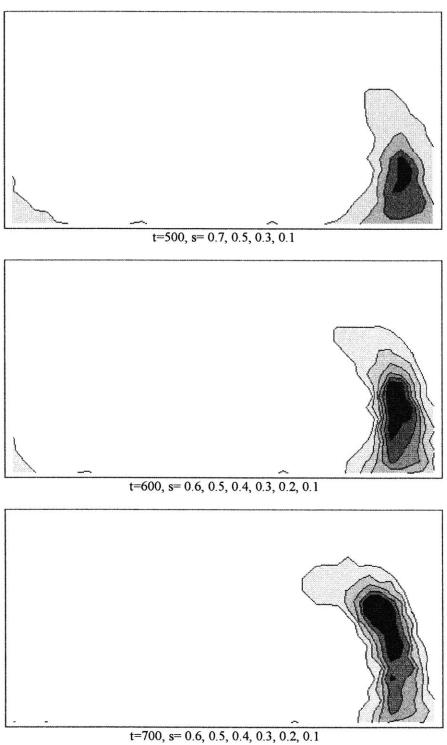
This experiment is similar to the first one but $\varepsilon=0.1$. This implies a strong chaotic behavior but the system is still dominated by the main wave. The experiment was carried out only for 1200 time steps, but it should be enough to compare both experiments.

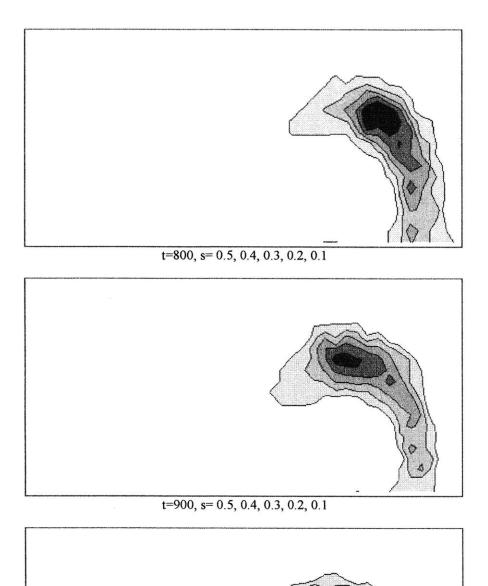




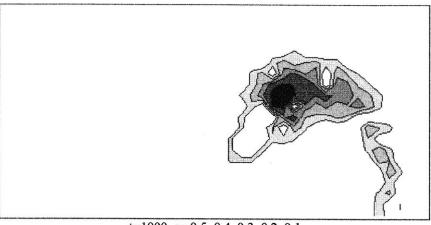
t=100, s= 0.9, 0.7, 0.5, 0.3, 0.1



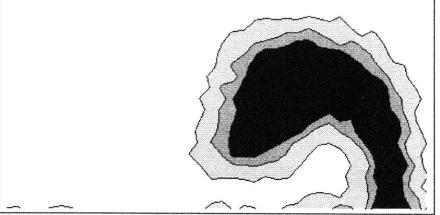




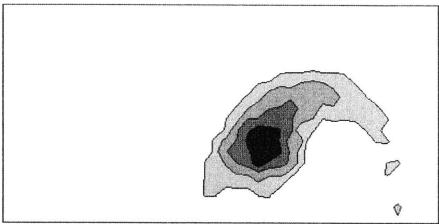
t=1000, s=0.5, 0.4, 0.3, 0.2, 0.1



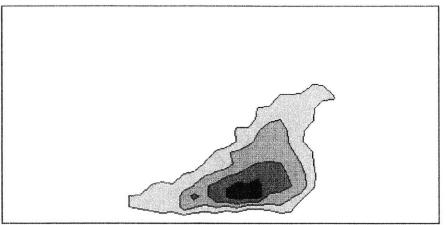
t=1000, s= 0.5, 0.4, 0.3, 0.2, 0.1 No smoothing



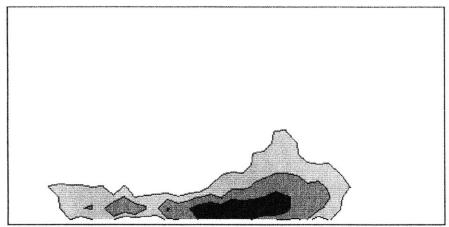
t=1000, s= 0.1, 0.05, 0.01



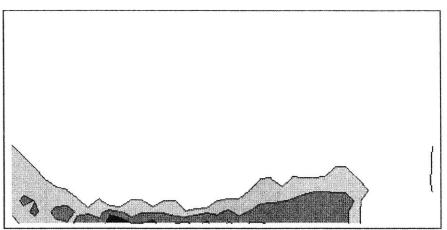
t=1200, s= 0.4, 0.3, 0.2, 0.1



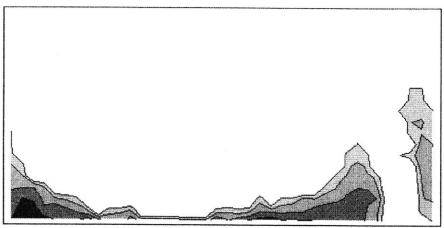
t=1400, s= 0.4, 0.3, 0.2, 0.1



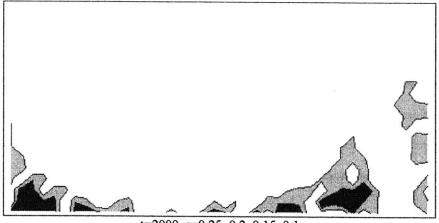
t=1600, s= 0.3, 0.2, 0.1



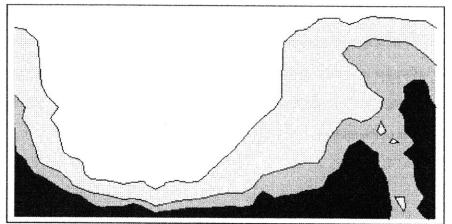
t=1800, s= 0.3, 0.2, 0.1



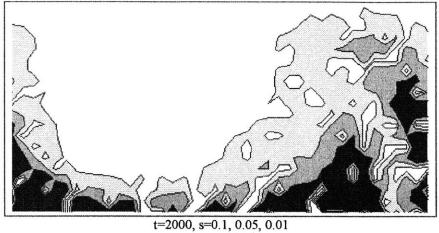
t=2000, s=0.25, 0.2, 0.15, 0.1



t=2000, s=0.25, 0.2, 0.15, 0.1 No smoothing



t=2000, s=0.1, 0.05, 0.01



No smoothing

The contours plotted without smoothing the grid show the smoothing process isn't altering the data significantly. The advection process is obviously dominating, but from the contours for smaller values it is evident the tracer is also diffusing slowly into the whole domain. This is also obvious from the need to use smaller and smaller values for the main contours. Of course, if instead of just having a fixed amount of tracer arranged in the initial state there was a steady source of tracer the levels of tracer in would increase slowly in the whole domain and eventually there would be a steady flux across the channel.

One obvious feature of this scheme is that on this non-chaotic system (or in one with a separatrix along the middle of the channel) the tracer should only be able to move to the north of the channel by diffusion. Given a small value for the diffusion constant this should be quite a slow process. In a grid model this is not true. As discussed before the separatrix cannot be modeled easily and hence there is always a small but significant advection departing from the behavior given by the stream function – since the velocities are averages over a small section of the channel.

This second experiment show a much stronger diffusive behavior than the first one. This must be a direct result of the chaotic behavior of the system. This seems plausible if chaos tends to extend in filaments the tracer over large areas (filaments in turn enhance diffusion), as suggested by *Pierrehumbert (1991)*.

It is however difficult to make conclusions from only two experiments with such low resolution. One of the main drawbacks of this kind of model is that it is (at least as I implemented it) much more time consuming than a grid model. First there is the integration of the particle trajectories, then the rearranging in time steps, then the sorting by coordinates and finally the interaction between particles. Even the last step can be more time consuming than a simple grid model. Needless to say increasing the resolution is very hard without taking the computing time to unmanageable levels. A useful experiment would also need to be carried on for a much longer time (until a steady state is reached).

Even if this was not a problem there are other kinds of problems. One that can be appreciated from the particles positions is that there are gaps left between the particles of very different sizes and that can appear almost anywhere in the channel given enough time. Dealing with this problem is not easy at all. Particles that are bunched together interact strongly while particles on a more sparsely populated area interact weakly (if at all). In principle, the density of the particles should remain equal to the density of the fluid around them, but if we track them independently this is not easy to accomplish. There is also no way of telling how bad the effect of these gaps is since one can correspond to an area with strong or weak advection and strong or weak tracer gradients. There are a number of variations of this model that could be tried. An hybrid model where particles interact with cells of a grid instead of other particles (also without cell to cell interaction), or one where particles carried the advection and cells the diffusion are certainly feasible. New particles could be added after each iteration to fill the gaps while removing some from more dense areas. With the help of a grid the position of the particles could be reset after each iteration (or after a few) to cover the channel uniformly. How would the initial distribution affect the outcome in that case? However it is not clear if any of these models could actually solve all the problems of grid and Lagrangian models or if they would have the problems of both.

Grid Experiment.

The next step was to use an Eulerian approach, through a grid model, hoping this simple model could reflect the effects of chaotic behavior in our system. Such model has several advantages, including simpler numerical calculations, consequently faster computations and also a Newtonian diffusion scheme which is generally accepted (although sometimes reluctantly) to describe the diffusive dispersion of a tracer on a fluid.

The model is very simple and corresponds to a differential equation of the form:

$$\frac{\partial S}{\partial t} + u \frac{\partial S}{\partial x} + v \frac{\partial S}{\partial y} = K \frac{\partial^2 S}{\partial \vec{x}^2}$$

Then I discretized the differential equation the following way:

$$\frac{\Delta S}{\Delta t} + u_i \frac{\Delta S}{\Delta x} + v_i \frac{\Delta S}{\Delta x} = K \frac{\Delta S}{(\Delta x)^2}$$

Since $\Delta x = \Delta y$. The ΔS however means different things in each term of the equation. More explicitly:

$$\frac{S_{i,j}(t+1) - S_{i,j}(t)}{\Delta t} + u_{i,j,+} \frac{S_{l+}}{\Delta x} + u_{i,j,-} \frac{S_{l-}}{\Delta x} + v_{i,j,+} \frac{S_{m+}}{\Delta x} + v_{i,j,-} \frac{S_{m-}}{\Delta x}$$
$$= -K \frac{(4S_{i,j}(t) - S_{i+1,j}(t) - S_{i,j+1}(t) - S_{i,j+1}(t) - S_{i,j-1}(t))}{(\Delta x)^2}$$

Where the diffusive term was transformed just using first differences and the advective terms as in a box model. The velocities (+) correspond to the north and east edges of the grid cell and the velocities (-) correspond to the south and west edges of the grid cell. The corresponding values of S are either the value on the cell we're working with if the velocity is going outward, or the value of the neighbor cell if the velocity is going inward.

What we're really interested in is the value of S after one time step; then we can solve the equation explicitly for this value:

$$S_{i,j}(t+1) = S_{i,j}(t) - u_{i,j,+}S_{l+}\frac{\Delta t}{\Delta x} - u_{i,j,-}S_{l-}\frac{\Delta t}{\Delta x} - v_{i,j,+}S_{m+}\frac{\Delta t}{\Delta x} - v_{i,j,-}S_{m-}\frac{\Delta t}{\Delta x} - K(4S_{i,j}(t) - S_{i+1,j}(t) - S_{i,j+1}(t) - S_{i,j+1}(t))\frac{\Delta t}{(\Delta x)^2}$$

This is like a 2^{nd} upwind differencing scheme. The next concern is calculating an optimal time step. Obviously this time step depends directly on Δt and Δx , but also on the size of u and v (which vary from cell to cell and depend on the size of the grid). The values of the velocities are actually an average on the corresponding side of the cell. Since the velocities come from the stream function, they are just:

$$u_{i,j,+} = \frac{1}{\Delta x} \int \Psi((i+1)\frac{\pi}{N}, y) = \frac{\Psi((i+1)\frac{\pi}{N}, (j+1)\frac{\pi}{N}) - \Psi((i+1)\frac{\pi}{N}, j\frac{\pi}{N})}{\Delta x}$$

With something equivalent for the other velocities, and the streamfunction. The streamfunction is:

$$\Psi(x, y, t) = \frac{1}{\sqrt{1+16\varepsilon^2}} [\sin(x)\sin(y) + \varepsilon\sin(4x + (c-c_2)t)\sin(4y)] + cy$$

From the norm it is obvious the value of the streamfunction has a maximum when $\epsilon \rightarrow 0$. The streamfunction can't be more than:

$$\Psi(\frac{\pi}{2}, y) = \sin(y) + cy$$

And the maximum velocity can be obtained the following way:

$$u = \frac{1+4\varepsilon}{\sqrt{1+16\varepsilon^2}} + c$$

If we differentiate with respect to ϵ to obtain the maximum:

$$\frac{4}{\sqrt{1+16\varepsilon e^2}} - \frac{16\varepsilon(1+4\varepsilon)}{(1+16\varepsilon e^2)^{\frac{3}{2}}} = 0$$

$$4(1+16\varepsilon^{2}) = 16\varepsilon(1+4\varepsilon)$$
$$\varepsilon = \frac{1}{4}$$

And the maximum u is then:

$$u_{MAX} = \frac{2}{\sqrt{2}} + c = \sqrt{2} + c \approx 1.914$$

From the advective terms then we estimate an optimum time step as:

$$\Delta t = \frac{\Delta s \Delta x}{uS} \approx 0.5 \frac{\pi}{1.5N} \approx \frac{1}{N}$$

Considering a maximum $\Delta S = 0.5$, S = 1 and u = 1.5.

Most of the time the velocity is quite smaller and S is more likely around 0.5 so we will get a much smaller change in S. If we consider now the optimum time step for the diffusive term:

$$\Delta t = \frac{\Delta S (\Delta x)^2}{4K} = \frac{\Delta S \pi^2}{KN^2}$$

We can use this to choose a K such that the diffusive term will be competitive with the advective terms:

$$K = \frac{\Delta S \pi^2}{\Delta t N^2} \approx \frac{\pi^2}{2N} \approx 0.0658$$

This sets a maximum to the value of K we can work with consistently with the previous estimate of the time step; however a more sensible choice considering a change in S of around 5% per time step gives a value of K around 0.0025.

This immediately raises a couple of questions about this model. What is the model sensitivity to the size of the time step? And, what is the model sensitivity to the resolution of the grid? Since we found out the optimum time step is the inverse of the resolution (1/N) this two questions are intimately related. But even if the model proves to be sensitive to these two parameters, the behavior must be similar when we keep the grid fixed and change K and ϵ within a certain range. The normalization in principle assures we can choose safely any ϵ . When $\epsilon \rightarrow 0$, the model approaches a mode-1 wave with little chaos in it. When $\epsilon \rightarrow \infty$ the model approaches a mode-4 wave, again with little chaotic behavior. As shown in the first section of this work, the system seems to be more chaotic around $\epsilon = 0.25$ corresponding to the maximum velocity as well.

Boundary conditions.

In the continuous system the boundary conditions imply $\Psi = 0$ at the boundaries at y = 0 and $y = \pi$. The other boundary conditions are that the concentration of the tracer S = 1 at y = 0 and S = 0 at $y = \pi$. In the discretized system we have to transform these conditions in some other way, since the grid cells on the boundary represent not only the punctual position exactly on the wall of the channel but also the small adjacent area encompassed by the grid cells.

The boundary conditions for the grid experiment were:

(a)
$$y = 0$$
 $S_{i,0} = 2 - S_{i,1}$

(a)
$$y = \pi$$
 $S_{i,N+1} = -S_{i,N}$

Where $S_{i,0}$ and $S_{i,N+1}$ are outside the channel and serve to provide the boundary conditions, and $S_{i,1}$ and $S_{i,N}$ are inside the channel and calculated normally according to the model. These are set so the linear interpolation between the values of both adjacent cells provide a value of S = 1 at y = 0 and S = 0 at y = π .

This also implies there is no normal flow across the boundary but there is advection along the cells in the boundary.

Normalization in the grid.

So far I have been using a normalized stream function that assures a constant energy in the system (for different values of ε). The norm was $\sqrt{1+16\varepsilon^2}$. This works fine when working analytically. However, when working numerically on a grid we are approximating the continuous system. This introduces a margin of error that accumulated over the entire grid can produce slightly different values for the total energy of the system (depending on the resolution). Consider the following values:

ε=0.01	ε=0.1	ε=1.0	ε=10.0	ε=100.0
0.99990019472317	0.99970105080814	0.99852774171817	0.99844272994150	0.99844182669703

The difference between $\varepsilon = 0.01$ and $\varepsilon = 100.0$ is less than 0.0016. It is not certain this error accumulates over the time (the system takes around 15,000 iterations to reach the steady state). However since this problem is easy to avoid I added a numerical normalization procedure.

The idea is to find a new value for the norm such that the total energy when calculated numerically will add

up to exactly $\frac{3}{2}\pi^2$. The total energy is

$$\sum_{i}\sum_{j}(u_{i,j}^{2}+v_{i,j}^{2})\Delta x\Delta y = Energy$$

If we define the non-normalized, static frame stream function as:

$$\Phi(x, y, t) = \sin(x)\sin(y) + \varepsilon\sin(4x + (c - c_2)t)\sin(4y)$$

$$u_{i,j} = \frac{1}{\Delta y} [\Psi(i\Delta x, (j+1)\Delta y, t) - \Psi(i\Delta x, j\Delta y, t)] = \frac{\pi}{\Delta y \cdot norm} [\Phi(i\Delta x, (j+1)\Delta y, t) - \Phi(i\Delta x, j\Delta y, t)] + c$$

$$v_{i,j} = \frac{1}{\Delta x} [\Psi((i+1)\Delta x, j\Delta y, t) - \Psi(i\Delta x, j\Delta y, t)] = \frac{\pi}{\Delta x \cdot norm} [\Phi((i+1)\Delta x, j\Delta y, t) - \Phi(i\Delta x, j\Delta y, t)]$$

After doing the summation we will obtain an expression of the form:

$$\pi^{2}(\frac{A}{norm^{2}} + \frac{B}{norm} + C) = Energy$$

Where, assuming $\Delta x = \Delta y$:

$$A = \sum_{i} \sum_{j} \left[\Phi(i\Delta x, (j+1)\Delta y, t) - \Phi(i\Delta x, j\Delta y, t) \right]^2 + \left[\Phi((i+1)\Delta x, j\Delta y, t) - \Phi(i\Delta x, j\Delta y, t) \right]^2$$

It can be shown that B = 0, and $C = 2c^2$. Therefore the new norm should be:

Norm =
$$\sqrt{\frac{A}{(1+2c^2-2c^2)}} = \sqrt{A}$$

First set of experiments.

Using the model described before and the calculations for the optimum time step and size of the diffusive constant I did a first set of numerical experiments. The results are presented in the following tables. The first table presents the flux as the Nusselt number, which corresponds in this case to the ratio between the actual flux and the purely diffusive flux. In these first tables the rows represent different diffusive constants and the columns different values of ε .

Nusselt Number

	0.01	0.1	0.5	1	10	100
0.0005	161.854	174.0676	195.6724	185.5428	126.8689	123.6562
0.0015	75.99905	81.56299	91.10799	84.1424	61.22661	60.41056
0.0025	54.45467	57.90658	63.61464	58.22931	44.77147	44.38576
0.0075	29.86633	30.94495	32.36686	29.47908	25.35647	25.27894
0.0125	24.21834	24.8062	25.23771	23.07872	20.62391	20.58387

Flux / Time Unit

	0.01	0.1	0.5	1	10	100
0.0005	4.029087	4.333125	4.870941	4.61878	3.158191	3.078216
0.0015	5.936296	6.370897	7.116458	6.572375	4.782419	4.718677
0.0025	7.184139	7.639545	8.392602	7.682123	5.906646	5.85576
0.0075	12.04709	12.48217	13.05573	11.89089	10.22797	10.19669
0.0125	16.37468	16.77215	17.0639	15.60415	13.94438	13.91731

Time to reach steady state. (Final tracer input is shown if steady state was not reached)

	0.01	0.1	0.5	1	10	100
0.0005	0.013448	0.010371	0.007419	0.007912	0.01288	0.01329
0.0015	0.001292	472.347	438.347	461.013	0.001585	0.001649
0.0025	412.013	375.347	357.68	383.013	439.013	441.013
0.0075	236.347	218.347	223.68	246.013	270.013	270.347
0.0125	176.68	164.68	173.68	191.347	206.347	206.347

	0.01	0.1	0.5	1	10	100
0.0005	5488.99	5529.16	5562.91	5557.39	5493.24	5487.17
0.0015	5617.67	5621.62	5623.25	5622.23	5615.46	5614.99
0.0025	5624.05	5624.65	5624.79	5624.54	5623.17	5623.09
0.0075	5625	5625	5625	5625	5625	5625
0.0125	5625	5625	5625	5625	5625	5625

Tracer amount at the end of the experiment (t = 500)

The following table gives more values for K = 0.0025

	0.01	0.1	0.5	1	5	10	100	1000000
Nusselt	54.45467	57.90658	63.61464	58.22931	45.84942	44.77147	44.38576	44.38151
Flux	7.184139	7.639545	8.392602	7.682123	6.048859	5.906646	5.85576	5.855199
Time	412.013	375.347	357.68	383.013	433.68	439.013	441.013	441.013
Tracer	5624.05	5624.65	5624.79	5624.54	5623.36	5623.17	5623.09	5623.09

There are several points to be made from these tables. First, and addressing the question I'm trying to answer in this work, I'd like to know if there is indeed any indication of an increased flux when the system is more chaotic. The answer seems to be yes. The maximum fluxes are found for $\varepsilon = 0.5$ where the system is clearly not dominated by either of the 2 modes, and hence the particles are in their most chaotic behavior. The mode-1 wave also seems to be much more transportive than the mode-4 wave. This evidently is a result of creating zones with stronger tracer gradients, which promote stronger diffusion.

How good are these experiments though? When I described this model I posed a couple of questions. What is the model sensitivity to the size of the time step? What is the model sensitivity to the resolution of the grid? Also, since I'm only using first differences to approximate the velocities, how big is the numerical error?

After exploring these issues I found out there is indeed a strong numerical diffusivity associated with this model. The resolution issue is intimately related. In the next pages I discuss these problems.

Numerical Diffusion.

Lets examine the model to try to estimate the error associated with it. For simplicity I will look only at the one-dimensional problem. Just taking the advective terms:

$$S(t + \Delta t) - S(t) = -\frac{\Delta t}{\Delta x} (u_R S_R - u_L S_L)$$

Suppose U_R , $U_L > 0$, then:

$$S(t + \Delta t) - S(t) = -\frac{\Delta t}{\Delta x} (u_R S_i - u_L S_{i-1})$$

Approximate the velocities at the edge of the cell by a simple average of the velocities in the center of the cells (remember however that I am calculating directly the velocities in the edges):

$$u_{R} = \frac{1}{2}(u_{i+1} + u_{i}) \qquad u_{L} = \frac{1}{2}(u_{i} + u_{i-1})$$
$$S(t + \Delta t) - S(t) = -\frac{\Delta t}{\Delta x}(\frac{1}{2}u_{i+1}S_{i} + \frac{1}{2}u_{i}(S_{i} - S_{i-1}) - \frac{1}{2}u_{i-1}S_{i-1})$$

Now use a Taylor expansion for the values $S(t+\Delta t)$, $S(x\pm\Delta x)$, $u(x\pm\Delta x)$.

$$S_{i+1} = S(x + \Delta x) = S(x) + \Delta x \frac{\partial S(x)}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 S(x)}{\partial x^2} + \dots$$

$$S(t + \Delta t) = S(t) + \Delta t \frac{\partial S(t)}{\partial t} + \frac{(\Delta t)^2}{2} \frac{\partial^2 S(t)}{\partial t^2} + \dots$$

$$S_{i-1} = S(x - \Delta x) = S(x) - \Delta x \frac{\partial S(x)}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 S(x)}{\partial x^2} + \dots$$

$$u_{i+1} = u(x + \Delta x) = u(x) + \Delta x \frac{\partial u(x)}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u(x)}{\partial x^2} + \dots$$

$$u_{i-1} = u(x - \Delta x) = u(x) - \Delta x \frac{\partial u(x)}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 u(x)}{\partial x^2} + \dots$$

If we replace this values on the former equation ignoring terms of higher orders than $(\Delta x)^2$, as well as some of the cross-products:

$$\frac{\partial S}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 S}{\partial t^2} = \frac{-1}{2\Delta x} \left[uS + \Delta x \frac{\partial u}{\partial x} S + \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} S + uS - uS + u\Delta x \frac{\partial S}{\partial x} - u \frac{(\Delta x)^2}{2} \frac{\partial^2 S}{\partial x^2} - uS + \Delta x u \frac{\partial S}{\partial x} - u \frac{(\Delta x)^2}{2} \frac{\partial^2 S}{\partial x^2} + \Delta x \frac{\partial u}{\partial x} S - \frac{(\Delta x)^2}{2} \frac{\partial^2 u}{\partial x^2} S \right]$$

Eliminating terms:

$$\frac{\partial S}{\partial t} = -\frac{\partial (uS)}{\partial x} + u \frac{\Delta x}{2} \frac{\partial^2 S}{\partial x^2} - \frac{\Delta t}{2} \frac{\partial^2 S}{\partial t^2}$$

If we treat the velocity as a constant we can write:

$$\frac{\partial S}{\partial t} = -u\frac{\partial S}{\partial x} + u\frac{\Delta x}{2}\frac{\partial^2 S}{\partial x^2} - \frac{\Delta t}{2}\frac{\partial^2 S}{\partial t^2}$$

But the correct relationship is actually:

$$\frac{\partial S}{\partial t} = -u \frac{\partial S}{\partial x}$$

Then, if we continue to treat the velocity as constant it follows:

$$\frac{\partial^2 S}{\partial t^2} = \frac{\partial}{\partial t} \left(\frac{\partial S}{\partial t} \right) = -u \frac{\partial}{\partial t} \left(\frac{\partial S}{\partial x} \right) = u^2 \frac{\partial^2 S}{\partial x^2}$$
$$\frac{\partial S}{\partial t} = -u \frac{\partial S}{\partial x} + u \frac{\Delta x}{2} \frac{\partial^2 S}{\partial x^2} - \frac{u^2 \Delta t}{2} \frac{\partial^2 S}{\partial x^2}$$

And you can see, besides the advective term (the first one), we have introduced two diffusion-like terms, one depending on the time step and the other on the resolution of the grid. We can define two numerical diffusion parameters to compare its magnitude to that of the diffusive constant.

$$K_x = \frac{u\Delta x}{2}$$
$$K_t = -\frac{u^2\Delta t}{2}$$

The other thing to remember are the stability conditions:

$$\frac{u\Delta t}{\Delta x} \le \frac{1}{2}$$
$$\frac{4K\Delta t}{\Delta x^2} \le \frac{1}{2}$$

Which follow from the equation for the model to avoid taking out of a cell more than the amount of tracer in it. Of course the smaller these two products are the better the model will behave, but also keep in mind the velocity in the first product is the maximum velocity.

Calculating these diffusion constants from the values I have been using so far (assume u = 1) we get the following:

$$\mathbf{K} = 0.0005 - 0.0125$$

 $K_x \approx 0.021$

 $K_{t} \approx 0.0067$

As you can see, the term associated with the time step is small (although still larger than the smallest diffusive constants used, but smaller than Kx in any event), the term associated with the grid resolution is larger than any of the diffusive constants used though. Is there a reasonable choice of values we can make to keep working with this model and get reasonable answers?

Let's start by making K_x small compared to the diffusive constant:

$$\frac{u\Delta x}{2} = \frac{K}{10}$$
$$\Delta x = \frac{K}{5}$$
$$\frac{4K\Delta t}{K^2/25} \le \frac{1}{2}$$
$$\frac{100\Delta t}{K} \le \frac{1}{2}$$

Now, assuming for example K = 0.0025 = 1/400, then we get:

$$\Delta t \leq \frac{1}{80000}$$

compared to the value 1/75 I used for the first set of experiments. This time step is far too small to use in any simulation with the resources I had at hand; however, the only assumption made in the process was choosing a diffusion constant and setting the resolution is such a way as to make the numerical diffusion small compared to it. There are a few ways to get around this problem though. First a compromise has to be reached between making the numerical diffusion small and having an acceptable resolution and time step. With this in mind I chose to use a value of K=0.035 for the next series of experiments. This means the Reynolds number of the cell will be large since there is no way to make the advection as strong as the diffusion locally and still keep the numerical diffusion small. In the whole domain, though, the advection remains the most important process in the transport of the tracer, as will be seen from the Nusselt numbers obtained in the following experiments.

Optimal resolution.

The question of what time step and resolution to use exactly remains to be answered. To find out systematically which resolution would be good enough to obtain reasonable results, despite the existence of a small amount of numerical diffusion, I ran a series of experiments using different resolutions. The diffusion constant used in all the experiments remained K = 0.035. Two sets of experiments were done, one using a pure mode-1 wave, and the other using a pure mode-4 wave.

The results are presented in the following table:

	150x75	200x100	250x125	300x150	450x225	600x300	750x375
Mode-1	34.28755	33.18715	32.50541	32.06861	31.64214	31.42093	31.31296
Mode-4	27.81121	27.14093	26.74575	26.46651	26.00121	25.74607	25.62017

The important point here is to observe how the value changes with the resolution. For very coarse resolutions the numerical diffusion is still important. For finer resolutions the numerical diffusion diminishes in importance and the flux across the channel is correspondingly smaller. The purpose of doing these sets of experiments was to find out at which resolution would the numerical diffusion no longer impact the flux very much. When going from resolution 450x225 to 600x300 the fluxes change less than 1%. For this reason the resolution 600x300 was chosen to carry out the last series of experiments in which the numerical diffusion is assumed to be no longer a problem.

Even at 600x300 the computational burden is considerable so different strategies to diminish the computer time were used. One of them was using as an initial condition for the experiments the steady state obtained from a low-resolution experiment. This procedure was refined using an algorithm to guess if the system would converge fast enough, and modifying it slightly otherwise. Since we are starting from a quasi-steady state in the experiment, we expect to see only small gradients in the distribution of the tracer. This means we can considerably relax the stability conditions since ΔS will no longer be order 1, but much smaller.

Last set of experiments.

Having chosen an optimal resolution of 600x300 cells, and a diffusion constant of K = 0.035, I could now proceed to repeat the kind of experiments done the first time (changing the size of the perturbation). Due to limited time I couldn't repeat these experiments using different diffusion constants, however I think there is enough evidence so far to assume the behavior doesn't really change significantly with different diffusion constants. The effect of altering the diffusion constant is the obvious one of increasing or decreasing a base level of transport on top of which the different advective processes modify the amount of this tracer transport.

The results of these experiments are presented in the following table:

	0	0.01	0.1	0.175	0.25	0.5	1	10 ⁹
Nusselt	2.474524	2.53379	2.603964	2.608708	2.55875	2.342921	2.161129	2.027606
Flux	31.42093	32.17349	33.06453	33.12478	32.49042	29.74988	27.44153	25.74607

We confirm from these experiments that the mode-1 wave is around 20% more transportive than the mode-4 wave, and there is a strong indication that the chaos resulting from the superposition of both waves increases the transport of tracer across the channel. Comparing these results with the first set of experiments using the grid it seems the maximum flux has slightly shifted towards the mode-1 wave and the maximum seems to be now around 0.175.

The evidence presented seems to support the hypothesis of Pierrehumbert that the chaotic mixing would spread the tracer more rapidly than a diffusive process, thereby facilitating the mixing of the tracer. In the system, I have discussed in this work, the enhanced mixing manifests itself as an increased tracer flux across the channel; however, the increase is only on the order of 10%.

Conclusions.

The experiments presented in this work seem to suggest the chaotic behavior does improve the flux across the channel. The effect however seems to be rather small. If we compare the highest flux obtained from the last set of experiments with the pure mode-1 wave flux the change isn't much more than 5%. The first experiments suggest the chaotic behavior will ensure the system reaches a steady state a little faster, but then again the effect isn't very significant when the times are compared to the pure mode-1 wave system.

The very simple system used in this work can be compared to several features in the ocean. Think of it for example as the boundary between two gyres and then the tracer can be a property such as temperature or salinity. This would then suggest the stronger chaotic behavior associated with a weak current (such as one that can be modeled by Rossby waves) will not significantly improve the cross-basin flux of the tracer, unless a change of 5% is important enough in our system to take it into consideration.

There are many questions left unanswered by this work of course. Will a Lagrangian model show a stronger effect of chaos? My guess is it probably will, however it is not easy or evident how to create such a model that might be able to accurately describe the distribution of a given property in the fluid as a whole and more importantly of its evolution. The Eulerian grid-model used for most of this work is well suited to describe such a distribution, however the effects of the chaotic behavior might be greatly reduced by reducing the many parts of the whole to an array of cells. Another issue is if there is a distinction between the superposition of the waves and the chaotic behavior produced by it, in a Lagrangian frame they are clearly undistinguishable, but is that also true in an Eulerian frame?

The effects of chaos are always there when we have a system with chaotic behavior, and that is almost always the case, the only question is how important are they? In the system studied in this work the answer is around 5% at most, keeping in mind this is true if we work from an Eulerian point of view.

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