* I want to talk to you about some of the research I’ve been working on for the last year with Jim. The ultimate aim of this work is to model the problem of in situ groundwater remediation, when there is a random distribution of sediment in an aquifer. Modeling spatially random processes in nonlinear systems like one-dimensional maps is not as popularly studied as the time-dependent case, so this work offers a slightly different view on some well-known maps, such as the logistic map and the circle map. A spatially random process is one that depends on space and is invariant in time; there is no time dependence in the process. So if you would imagine a function that takes on a different value for any given location in space, but retains the same value if it were to return to this same location at a later time, this function would be a spatially random process.
* This is the overall structure of my talk. I’ll walk you through the motivation for this work, touch on the analytic underpinnings of the numerical simulation, and discuss the results of the models.
* Like I previously mentioned, the aim of this work is to remediate contaminated groundwater. This plot tries to give you a sense of groundwater use in the US. The two main applications are in irrigation and in the public supply, which is drinking water.
* By nature of being underground, groundwater is highly susceptible to contaminants. You might think of runoff from mining operations or fertilizers and pesticides from farms leeching into the aquifer. In many cases, remediation requires injecting the aquifer with a treatment solution to break down the toxins. The treatment solution is only effective if it is thoroughly mixed with the contaminated water, so essentially this problem boils down to that of mixing, a favorite topic in nonlinear dynamics. However, there are more factors that impact the fluid flow underground than on the surface.
* The main factor is the type of sediment found in the aquifer because different kinds of sediment hold and release water in various capacities. For example, this table demonstrates the porosity and hydraulic conductivity of three kinds of materials: clay, sand, and gravel. Porosity is a measure of the fraction of empty spaces between particles and hydraulic conductivity is a measure of how easily water moves through the open pores. For instance, clay is highly porous, but has low hydraulic conductivity. This implies that a segment of aquifer primarily composed of clay may hold a lot of water, but the water would pass through this region very slowly. Now consider a region made of gravel. Fluid would pass through this region orders of magnitude faster. You can see there is very wide range of possible behaviors, depending on sediment type. Without the use of sophisticated equipment to detect the nature of the sediment in an aquifer, one might consider the distribution of materials as a random field. So, as contaminated water or treatment solution moves through the aquifer, it has to move around a randomly distributed field of obstacles.
* I like to think of the two solutions as colors of paint getting mixed together. The onset of chaos would result in a mixture that has a uniform color throughout. Before this state, the solutions would swirl, much like in this image. The onset of chaos is a positive sign because it indicates the interface length between the two solutions is very large, so we have degredation of contaminants.
* So now we have the main points of the analytic model. We want to simulate transmissivity in the model as a random function of space, and observations in the field suggest transmissivty follows a log-normal distribution. We also simplify the problem by reducing the dimensions from three to one, in order to lay the preliminary groundwork of studying spatial perturbations in a deterministic system. A future work would generalize the results of this investigation to higher dimensions. That is, think of the fluid flow in the aquifer as a 1-d map, and injection of treatment as the initial condition imposed on the map.
* Like I just mentioned, we want to make sure the spatially random processes in the model mimic the observed noise in aquifers. It should be log-normal. Furthermore, in aquifers, porosity in a neighborhood of rock tends to be somewhat consistent (highly correlated), whereas porosity between two areas on opposite ends of the aquifer can be completely different. Thus, the noise in the random process should depend on the distance between two locations instead of the locations themselves, and we call this property homogeneity.
* R(x) represents the log-normal random function of space, so this implies the xi(x) is a normal random function of space. A normally distributed random variable comes from a distribution where the mean and variance are given. In our model, we want the mean of xi(x) to be a constant, ln(r ), and the variance of the distribution, at this point, is a free parameter. One way to construct a function that is normal and has mean value ln(r ) is by using a Fourier series, where the magnitudes of the modes are independent but not identically distributed random variables, who may or may not be normal. To preserve the property of the mean value of xi(x), we can force the mean value of the modes to be zero, and for the sum to converge, the variance of the modes should fall off exponentially. The exponential decay in the variance of the modes has two parameters: alpha and L. alpha is a positive real constant, and L represents the correlation length. You can see that fixing a large L would make the magnitudes of the Fourier modes shrink, and small values of L allow more noise in the process.
  + The correlation length in the variance of the Fourier modes is also reflected in the variance of the overall process. The variance of the Fourier modes is the spectral density, and the Fourier transform of spectral density is defined as the covariance of the spatially random process xi(x). Based on this choice of S(n), small L will increase the range of values the correlation function of xi(x), and large L will reduce this range. In other words, small L 🡪 more variance in xi(x) and large L 🡪 less variance in xi(x).
* I’m going to reiterate that we are modeling the fluid flow in the system as a one dimensional map that is perturbed by these random fluctuations. One dimensional maps, despite being simple in construction, can exhibit chaotic behavior.
* At this point, I’d like to offer an interpretation of what chaos means. Essentially, it refers to a state of a system where there is no detectable pattern in its long-term behavior, but the behavior is highly dependent on how you start the system.
* The system I’m referring to is a function of space, x, and the long term behavior of the system can be found by iterating the map until the iterates in x converge to a single value (called a fixed point) or a set of values (called an orbit).
* One type of map is the logistic map, which is often used in population modeling. This map has one parameter, r, which needs to live in the interval between 0 and 4 so that iterates stay in the range [0,1]. The randomized logistic map would replace this constant parameter with a function of space, R(x). This function is also subject to the same requirements of r, that is, it must be bounded in 0,4. So then, R(x) must be based on a bounded distribution, such as the uniform distribution. Unfortunately I was unable to show that the sum of N uniform random variables that are independent but non-identical is normally distributed, so xi(x) might not be a log-normal process. Although, some numerical simulations of the process suggest it mimics the log-normal distribution.
* After doing some algebra and simplification, we find that the standard deviation of the random process must live in this interval so that R(x) < 4. Thus, the parameter that has the most impact on the magnitude of the Fourier modes in the random logistic map is the standard deviation of the spatial process, xi(x), which we can adjust within this range. You can see there is r and L dependence in this upper bound, so we have two knobs we can turn to control the magnitude of the random process.
* These orbit diagrams demonstrate where stable fixed points of the system are. The blue lines are the maps, the red line is the line where the subsequent iterate is equal to the current iterate, and the green lines show the trajectories of the orbits settling down. You can see that for the same value of r, there can be very different dynamics between the deterministic and the random map. The smoother picture is the deterministic map, and it has converged to a stable period 2 orbit, which means there are two stable equilibrium points. The wigglier picture is the random map, and it has converged to a stable period 4 orbit, which means there are four stable equilibrium points. It should be known that this is just one instance of a random map, other realizations would take on different values, so the map would be wiggly in a slightly different way. However, for all iterates in time, this configuration stays constant.
* The circle map is the second map I have studied. Vladimir Arnold popularized the map when he was examining the dynamics of a kicked rotor. As you can see there are two parameters in this map, k and omega. K is the coupling strength, or in other words, the magnitude of the oscillation from the sine term. Omega is the parameter that I will replace with the random function of space, and it represents the natural frequency of the system, or in other words, a vertical shift in the map. The most useful feature of the circle map (for my purposes) is that its parameters are not as strictly defined as the logistic map; k and omega can take on a wider range of values. So the random function of space Omega(x) can be based on an unbounded distribution, like the Gaussian distribution. This is convenient because it is easily shown that the sum of N normal random variables that are independent and non-identical does follow a normal distribution, implying our spatially random process is log-normal.
* The spatially random process for this map is similar to the logistic map. We use omega in place of r, and we have more flexibility in choosing the standard deviation of xi(x). The parameters we can turn are alpha and L, and they impact the variance of the Fourier modes.
* These are another pair of orbit diagrams to highlight the differences between the deterministic system and the randomized system. As you can see, a small spatial perturbation throughout the map causes very different long term behavior.
* The orbit diagrams were useful in seeing the long term behavior of the system for one set of parameters, but if you wanted to see the dynamics overall, you would look at something called a bifurcation diagram. Bifurcation diagrams demonstrate the long term behavior of the system as a function of the parameters, so as you increase a parameter, you would plot the locations of the stable periodic orbits as a dependent variable.
* This is the bifurcation diagram of the deterministic logistic map, and as you can see for larger values of r we have a dense region of orbits. Chaos has been proven to occur for values of r in this space.
* This is the bifurcation diagram for the randomized logistic map. Since the parameter is now a random function of space, for any given value of r, we can have a range of possible behaviors. Each value of r was tested for $N\_{x\_0}$ initial conditions. The discretization of $r$ for the simulation is represented by the value $N\_r$, the number of subintervals. This plot is for 1.8 million simulations of the random map. If iterating the map for any given set of parameters resulted in finding no periodic orbit of period $p\_{max}$ or less, then no orbit is recorded in the bifurcation diagram. Otherwise, the orbit locations are plotted along the $y$-axis in the figures and color coded according to period. An unexpected result of the simulation is the presence of the stable periodic orbits in the right side of the diagram. In the deterministic case, this region was previously unstable. There are also stable high period orbits for small values of r. There are only period 1 orbits for these values of r in the deterministic map.
* Increasing the correlation length by a multiple of 9 preserves the region, but introduces a wider spread of types of orbits for small values of r. The newly stabilized region is also obscured by high period orbits.
* I experimented with halving the variance of the spatially random process from the previous figures, and found the stable low period orbits for $r \in [3,4]$ endure even when the noise is restricted.
* Further, it appears there are fewer stable high period orbits in this region where r < 3 when $\sigma$ is small.
* A way to quantify chaotic behavior is by calculating a quantity called the lyapunov exponent. A positive exponent is an indication of chaos, whereas a negative exponent corresponds to stable orbits.
* The exponent of the deterministic logistic map is on the left, and we see there is a point in r where stable behavior transitions to chaotic behavior, the Feigenbaum period doubling accumulation point. In the randomized case, the delimination is unclear. One feature of the exponents seems to be preserved, and that is the negative spike around r=3.8. The spike is likely due to construction of the variance of the random process, since we required R(x) to be bounded in [0,4]. We have the upper bound on the variance falling off as ln(4/r), so as r -> 4, the variance approaches zero very quickly. This would cause the random process to have a smaller effect on the map when r is close to 4, and we see evidence of that as the negative spike of this plot.
* An interesting direction to explore is the distribution of period in the randomized map. In other words, what kind of periodic orbits would one expect to see for a certain spatially random process? Since the process itself is random according to some distribution, it must affect the distribution of periodic orbits in the map.
* We looked at period distribution by simulating the random map 5,000 times. We took 10 random initial conditions and tested them 500 times each with a newly generated random process for given values of r and L. Periodicity was checked up to $p\_{max}=100$. The histograms count unique periodic orbits, so if two or more initial conditions under the same random process converged to the same periodic orbit, only one was counted.
* This histogram was generated for an r value in the neighborhood of the observed stable region from the randomized map. You can see the most dominant period is 2, and the general trend seems exponential. However, a log scale plot of this histogram reveals that the trend in the data is not linear, which means the period distribution is probably not exponential. The error bars represent the standard error in calculating the mean over a sample size of 5000.
* Since there are two parameters in the circle map, its bifurcation diagram is 2 dimensional. It is called the Arnold tongues, named for the triangular regions where stable behavior occurs. The colorbar to the side demonstrates the period of the orbit on the graph. For example, these dark green regions on the sides are where period 1 orbits occur, and the light green in the middle matches period 2 orbits. Each value of $k \in [0,1.5]$ and $\omega \in [0,1]$ was tested according to the discretization of 1,000 subintervals in both the k and omega directions. If iterating the map for any given set of parameters resulted in finding no periodic orbit of period $p\_{max}$ or less, then the pixel corresponding to this value of $(\omega, k)$ was colored black. Otherwise, the pixel for this $(\omega, k)$ pair was colored according to the orbit period.
* The randomized circle map has a bifurcation diagram that has almost no similarity to the deterministic case. You can see we have lost the shape of the tongues, and the diagram is now asymmetrical. There are also high period orbits in a region where there is typically only period 1 fixed points. The randomness appears to have an overall destabilizing effect on the dynamics of the map. This is for a correlation length L=0.1 and an alpha = 10e-5. You can also see evidence of stable high period orbits where we had period 1 in the deterministic map.
* Reducing alpha by ½ eliminates nearly all the high period orbits in the left side of the diagram. And there seems to be more variation in the type of periodic orbit throughout the diagram.
* For the alpha back to its larger value at 10e-5, the correlation length has been increased by a multiple of 3. It is now L=0.3. Some symmetry appears to be regained, however, there is a period 2 region that now appears where there should only be period 1 orbits on the right side of the diagram. Additionally, there are high period orbits in the center tongue. The period 4 region from the deterministic map looks like it has been stretched out in multiple places.
* Reducing alpha by ½ shrinks and shifts this region. It also removes the high period orbits in the center tongues, and the period 4 region continues to look stretched out.
* For a correlation length of L=0.5, the period 2 region disappears, and we see more symmetry and tongue-shape. Increasing L is increasing the exponential factor in the decay of the variance of the Fourier modes, so larger values of L will make the random map resemble the deterministic case.
* A comparison of the lyapunov exponent of the deterministic and random case partially confirms my suspicions of instability in the random map; nearly no features of the graph are preserved, and the high density of positive values indicates chaotic behavior. The exponent is calculated by fixing omega=0.8 and varying k over [0,5]. You can see that chaos only occurs when k > 1 for the deterministic map, but it can occur for k < 1 in the random map.
* This is another way to look at the lyapunov exponents’ dependence on omega. Here, k is fixed at 1.5. It is interesting that there is asymmetry here as well. The left and right sides of this graph are quite different for the random case, yet in the deterministic case there is symmetry.
* Just as we studied the histogram for the logistic map, we may get some ideas about period distribution by considering the associated histograms for the circle map. The dominant period is 5, followed by 10 and 15. The thing to note here is that though the period distribution seems to fall off exponentially, it is not exponential, since a log scale plot of the values from the histogram does not follow a linear shape.
* That concludes the main results from the numerical simulations.
* In all, we observed a stable low period region for large values of r when we introduced randomness, and this region was unstable except for windows of stability in the deterministic map.
* We also noticed a number of high period orbits when we turned the knob on the randomness for small r. These kinds of orbits disappeared when we reduced the standard deviation of xi(x) to half of the max value.
* And finally, looking at the histograms of unique periodic orbits for certain values of r gave us a clue that the distribution of period may be exponential. It also told us that the stable low period region is mostly period 2 orbits.
* In the circle map, there was the birth of a period 2 region for a particular correlation length. This period 2 region is usually period 1 in the deterministic map. But the region disappeared for L shifted from L=0.3 by 2/10.
* Next, we generally saw asymmetry in the diagrams of the Arnold tongues and Lyapunov exponents, especially for small L. This was different from the random logistic map because the bifurcation diagram of that random map still retained the general shape of the deterministic case. The asymmetry suggests the noise is destabilizing, but the presence of period 2 orbits for certain correlation lengths implies some stabilizing factor. It looks like there is a trade-off between stabilizing and destabilizing effects on the random map as the noise is increased.
* Looking at the histograms of observed frequency of periodic orbits suggests the distribution of period is not exponential, unlike the logistic map. This might explain why the results from these two maps are so different. The noise in the circle map is definitely log-normally distributed so I would consider the results from the study of the circle map to be more in line with the fluid model in the aquifer. However, the results from studying the logistic map were unexpected, and it would be interesting to study this map as well, even though it is not as relevant to the aquifer.
* So over this past year we got a lot of interesting findings, but I feel like we almost have more questions now than when we started. Here are some ideas I have going forward. First, the obvious thing is to look at higher dimensional maps by extending the study to 2-D maps. Two such examples are the Lotka-volterra system and the Henon map. The lotka-volterra system is a system of ODEs, so that is quite different from the discrete time maps we’ve been looking at, but since they are coupled differential equations, they are more relevant to the fluids model. Unlike discrete time maps, ODEs have limit cycles, so it would be interesting to consider the effect of the random process on existence and stability of these limit cycles. Closer to our study of 1D maps is the 2D Henon map.
* Next, I think we should try to formalize the basin of attraction for chaotic regions of the map. In other words, which set of initial conditions lead trajectories to chaotic behavior instead of stable orbits? This might give clues on how you would inject treatment in the aquifer to get the best (chaotic) mixing. There are some clues from our study of 1D maps, like in terms of where to start for the optimal correlation length. Since correlation length in an actual aquifer is fixed and nonvariable, this may imply that one should determine the correlation length for each aquifer before injecting it with treatment. The numerical simulations were highly sensitive to the correlation length, so optimal mixing is likely dependent on correlation length as well.
* And finally, a topic that kept resurfacing as we were simulating the maps was the question of generalizing the distribution of zeros of this function. The existence of a fixed point or periodic orbit depends on finding the roots of this equation, so solving this question would give us a formal notion of how many periodic orbits exist for any given map that’s been perturbed by a spatially random process.