
Interim Report

Mathematics of Planet Earth CDT

Manuel Santos Gutiérrez

Reading, March 2018

In the perturbation analysis of climate models and in general, statistical mechanical models, one has to consider two kinds of sensitivity. First, one has to take into account the dependence of the system on initial conditions often arising from basic assumptions of chaoticity. Secondly, the sensitivity to sudden changes in the parameters of the governing laws are to be studied. This is the problem to be tackled in this project. Based on response theory of statistical mechanical systems we shall make a transfer operator approach in order to extract the dynamical information and formulate a response theory based on this idea.

This document aims to give an overview of the work done in the first phase of the research project. The first section is devoted to give a review of the main texts and scientific articles that have been used as a foundation of the project. A schematic presentation of the theory and its references are given. A summary of the results obtained and the experiments performed will be done in the second section, to conclude with a final word on the prospects of the research.

Literature Review

Response theory was developed in the context of statistical mechanics as a tool to understand the behaviour of complex systems affected by perturbations. When the dynamics of the system is Hamiltonian, a first set of formulas were found [5] to describe the evolution of perturbations and the statistical properties of the system. It was not until 1997 when David Ruelle [18] established a mathematical framework to deal with response theory for a special class of dynamical systems where one gets that the invariant measure of the system is differentiable under changes in the perturbation control parameter.

One of the main problems in climate modelling is the investigation of the response to perturbations of external forcing. The dynamics of climate are far from being Hamiltonian or linear so the invariant measures of the system are not Gaussian, so it is necessary to construct an appropriate way of measuring and estimating the invariant measure of the system [15], [17]. Further, the perturbations in climate models can be non-infinitesimal. For this case, a response theory can be found in [22] with a special application to systems possessing fast-slow dynamics (see [10]).

Far from being a fixed, there are many approaches to response theory that depend on the character of the governing dynamics, for instance if the system is random or not [17]. It is the case that by analysing suitable operators one can extract information about the dynamics of the system and its statistical properties. These operators arise naturally from a given dynamical system and they describe the evolution of distributions and observables of the domain space. By looking at their spectrum one can compute the invariant measure of the system and infer other dynamical properties of it. This method has been used to study the response of dynamical systems by introducing perturbations directly into these operators and observing the change they provoke in their spectral properties [17], [2].

The Transfer Operator

Given a dynamical system S acting on some domain X , the *Koopman* operator $U : L^\infty \longrightarrow L^\infty$ as $\phi \mapsto \phi \circ S$ for any observable $\phi \in L^\infty$. The adjoint of this operator is the *transfer operator* [1], $T : L^1 \longrightarrow L^1$. Under absolute continuity conditions, L^1 could be identified with probability density functions, implying that T updates the initial probability distribution of the system to its density after the action of the dynamical system. Following the theory presented in [9], one can see that the operator norm of T is bounded by 1 and

that constant functions are eigenfunctions of T associated with the eigenvalue 1 which, by the spectral radius formula, the spectral radius of T is 1. Clearly, the invariant measure is precisely given by the eigenfunction associated to the eigenvalue 1.

The dynamics we want to study can be formally represented as:

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(\mathbf{x}), \quad (1)$$

where \mathbf{F} is the vector field acting on X . This equation induces a *flow* that we shall denote as $\{S^t\}_{t \geq 0}$, where S^t is a dynamical system on X and the whole set is a semigroup on $t \geq 0$. This way the transfer operator presented earlier has to be parametrised on t , i.e., T^t is a transfer operator for each t . Therefore, for each value of time $t \geq 0$, $T^t : L^1 \rightarrow L^1$ maps the initial probability distribution $\rho(\mathbf{x}, 0)$ to the probability distribution $\rho(\mathbf{x}, t)$ at time t . We could write this as:

$$\rho(\mathbf{x}, t) = T^t \rho(\mathbf{x}, 0). \quad (2)$$

Assuming that $\{T^t\}_{t \geq 0}$ is a C_0 -semigroup*, one can find a generator of this semigroup (usually closed and unbounded) called the Liouville operator \mathbf{L} ([14],[17]), such that,

$$\partial \rho(\mathbf{x}, t) = \mathbf{L} \rho(\mathbf{x}, 0). \quad (3)$$

Usually, $\mathbf{L}\psi = -\nabla \cdot (\psi \mathbf{F})$, where \mathbf{F} is the vector field governing the motion. The solution of (3) is formally given by $T^t = \exp(\mathbf{L}t)$. The foundations of these semigroup concepts lies within the Hille-Yoshida framework [16].

After iterating the dynamical system, the updated probability density function is determined by T^t , but, how fast does the system evolve towards the invariant measure? How fast is the *decay of correlations*? [1]. In general, one can only be sure of the exponential convergence in if the eigenvalue 1 is isolated from the rest of the spectrum, i.e., there is a *spectral gap*. This leads to the well posedness of the dynamical system in when it comes. Accordingly with the power method for matrices, the spectral gap determines the rate of decay of correlations in a statistical mechanical system.

The presence of a spectral gap is not obvious. It is always the case that the leading eigenvalue is 1 but maybe it is not isolated, leading to modulations in the decay of correlations [2]. A suitable choice of Banach space where to define T^t can be the solution to our problems in many cases. For instance, in one dimensional dynamical systems, if one is capable of finding an inequality like

$$\|Tf\|_A \leq r\|f\|_A + R\|f\|_B \quad (4)$$

for some norm $\|\cdot\|_A$ and seminorm $\|\cdot\|_B$, then there is a spectral gap REF. This inequality is called a Lasta-Yorke type of inequality. In [11] we find proves of this fact for a certain class of operators to eventually extend this result. The well-posedness of response theory relies on this idea.

Finite State Space Markov Chains

Although the response theory for a continuous dynamical system is formulated within an infinite state space, one would like to know how to compute the response of a dynamical system upon discretisation. In [14] a response theory for finite state space Markov processes is established and the basic response formulas are provided. Unlike earlier in this document, finite state Markov operator are precisely described in terms of stochastic

*Bounded for each t and strongly continuous.

matrices or Markov matrices. Let $\mathcal{M} \in \mathbb{R}^{n \times n}$ denote a Markov matrix. By definition, we have that $\mathcal{M}_{i,j} \geq 0$ for every $i, j = 1, \dots, N$ and

$$\sum_{j=1}^N \mathcal{M}_{i,j} = 1.$$

Note that the vector $[1, \dots, 1]$ is a left eigenvector of \mathcal{M} , therefore it is always the case that \mathcal{M} has an the eigenvalue 1. The invariant measure of the system is obtained by solving

$$\mathcal{M}\mathbf{u} = \mathbf{u} \quad (5)$$

which is equivalent to solving an eigenvalue problem for the eigenvalue 1. Perron-Frobenius theorem [9] cannot be strictly applied in this context unless one requires that $\mathcal{M}_{i,j} > 0$, so it is not clear, *a priori* wheter there are other eigenvalues in the unit circle in the complex plane.

Assuming the existence of a spectral gap, the second largest eigenvalue in modulus determines the rate of convergence to the invariant measure of the system. In other words it measures the convergence rate of the *power method* to compute the largest eigenvalue. Schematically written by

$$\lim_{n \rightarrow \infty} \mathcal{M}^n \mathbf{u}_0 = \mathbf{u}, \quad (6)$$

where $\mathbf{u}_0 \in \mathbb{R}^n$ is the initial density of the system and $\mathbf{u} \in \mathbb{R}^n$ is the same as in (5) up to a constant. A discussion on the importance of the second largest eigenvalue is found in [3] and [14].

Response Theory for Finite Markov Models

Consider a perturbation of the dynamics of the system given by:

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(\mathbf{x}) + \epsilon \mathbf{X}(\mathbf{x}). \quad (7)$$

This change in the dynamics induces a variation in the evolution of the probability density function.

$$\mathcal{M} \longrightarrow \mathcal{M} + \epsilon m. \quad (8)$$

Obviously, the perturbation considered preserves the Markovianity of transfer operator, so there some retrictions on the choice of m . However, 1 is still the largest eigenvalue of the system although the associated eigenvector might change. This is, if \mathbf{u} is as in (5), the eigenvector associated to 1 in the perturbed system \mathbf{v}_1 is given by

$$\mathbf{v}_1 = \mathbf{u}_1 + \sum_{n=1}^{\infty} \epsilon^n \prod_{k=0}^n \left(\sum_{m=0}^{\infty} \mathcal{M}^k m \right). \quad (9)$$

This formula establishes a response theory for finite state Markov operators and it is found in [14]. The series expansion in (9) is an algorithmic way of representing $(1 - \mathcal{M})^{-1}$ when $1 - \mathcal{M}$ is clearly uninvertible. This issue is addressed in [14] in the finite state case but extends to more complex situations in which \mathcal{M} is no longer a matrix but a general Markov operator. The remarkable point here is that the response is calculated at all orders of the perturbation.

Numerical Approximation of Transfer Operators

Finite state Markov models often arise as a discretisation of the transfer operator of a dynamical system. Ulam's method (REF) is a classical way of obtaining discrete approximation of the transfer operator of the dynamical system. By working on the phase space, one discretises the domain into connected (up to a measure zero intersection) boxes and analyses the proportion of each box visiting the remaining boxes. Formally, suppose that we split the phase space into N boxes $\{B_1, \dots, B_N\}$ and each box contains a pile of sand grains. Denote as $\eta(A)$ the number of sand grains in some set A . Then, the approximating matrix of the transfer operator is defined by

$$P_{i,j} = \frac{\eta(B_i \cap S^{-1}(B_j))}{\eta(B_i)}, \quad (10)$$

for $i, j = 1, \dots, N$. Clearly, $0 \leq P_{i,j} \leq 1$ and $\sum_j P_{i,j} = 1$ for every $i = 1, \dots, N$, meaning that the matrix P is, indeed, a stochastic matrix or a Markov matrix. This method of approximating the transfer operator is called *coarse graining*.

Another way of approximating the transfer operator is by starting running an initial integration of, say, M iterations and neglect the first few points (the first points are not populating the limiting set). Secondly we discretise the domain into boxes B_1, \dots, B_N and we classify each point according to what box they are in. Then, we calculate the amount of points in B_i that end up in B_j after one iteration. This method provides a very sparse approximation of the transfer operator and the invariant measure obtain using this method is fully supported in the attractor.

Numerical Experiments

In this section we will give an overview of the numerical experiments done and the computer resources used. The target at this stage was to be able to implement the coarse graining algorithm for discrete maps and simple sets of differential equations. Running the coarse graining produces an approximation of the transfer operator (a transition matrix) from which we calculated the dominant eigenvector to obtain the invariant measure, as explained earlier.

0.0.1 Hénon Map

The Hénon Map is a two dimensional discrete map which was studied by the french astronomer Michel Hénon [7]. This map was used as a model of a Poincaré section taken in Loren 63 [12]. The model is given by the following equations:

$$\begin{cases} x_{n+1} = 1 + y_n - ax_n^2 \\ y_{n+1} = bx_n \end{cases} \quad (11)$$

where $a > 0$ and $|b| < 1$. We performed Ulam's method to approximate the transfer operator associated with this set of difference equations. To do so, we ran a very long iteration of the vector field until we are certain that the trajectory has spent a long time within the attractor. After that we neglect the first few elements in the sequence, since there might be a delay before a trajectory enters the limiting set. Having discretised the domain into N boxes, we keep record of the amount of elements in the trajectory that populate each box. By construction this measure will be supported in the limiting set.

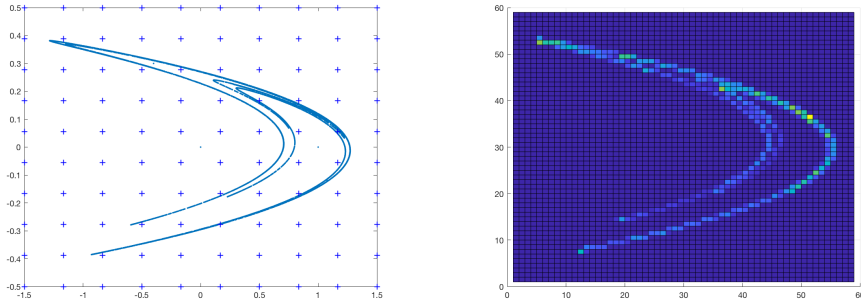


Figure 1: On the left we show the box discretisation of the phase space and a long run of the Hénon map taking $[0,0]$ as the initial condition. On the right there is a plot of the normalised invariant measure of the system where the yellow colours denote a concentration of mass

The spectrum of the transition matrix is given in Figure PPP. We observe that there is a spectral gap. Of course, this just means that this approximation of the transfer operator can be iterated and it will eventually converge. We also present a rough estimate of the generator of the transfer semigroup. We observe that this approximation matches the theoretical results that tell us that the spectrum should be contained in the left-hand-side of the complex plane. This is a confirmation of Hille-Yoshida theorem, which establishes the conditions by which an operator generates a semigroup. To obtain this estimate one has to take the formal logarithm of the transition matrix.

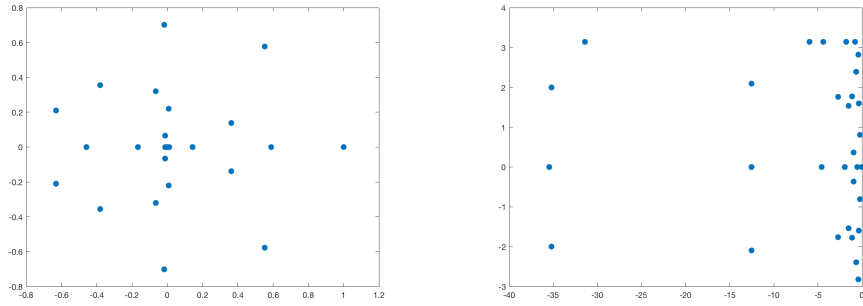


Figure 2: The first picture shows the spectrum of the transition matrix of the Hénon map. The second corresponds to the spectrum of the logarithm of the transition matrix.

0.0.2 Poincaré Section of Lorenz 84

Following the study of discrete maps, we consider now a new Poincaré section of the Lorenz 84 model [13]. To approximate the transfer operator we proceeded in the same way as before. By integrating the equations for long enough, we obtained a trajectory consisting of 649 points. To solve the equations numerically, we used the built-in MATLAB command `textode45`. In Figure 3 we observe a realisation of a trajectory and the domain divided into boxes of size 256 along with the invariant measure of the system.

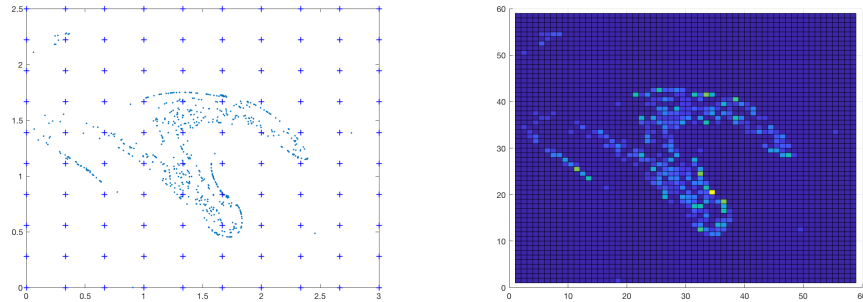


Figure 3: Normalised invariant density (right) and sample trajectory of the Poincaré section of Lorenz 84 (left).

The spectrum of the transition matrix computed for this discrete map shows, as in the previous case that this approximation has a spectral gap and therefore matrix power iterations will lead to exponentially fast convergence. We highlight that this does not show that the map is actually exponentially mixing.

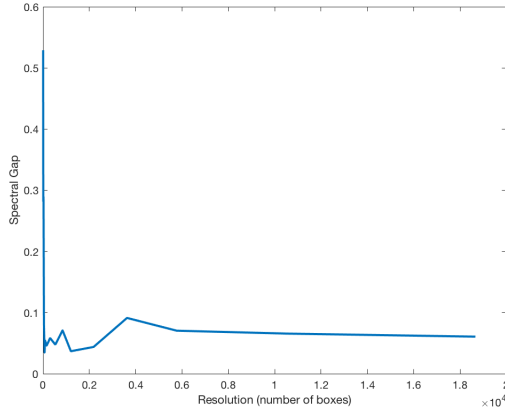


Figure 4: Spectrum of the transition matrix of the Poincaré section of Lorenz 84.

0.0.3 Lorenz 63

To implement Ulam's method for continuous dynamical systems we have used the MATLAB package GAIO REFERENCE. This package provides efficient tools to calculate the phase space discretisation and to obtain approximations of the unstable manifold of the system amongst other features. In this document, we present some experiments done using GAIO to calculate a box discretisation of the phase space and the calculation of the invariant measure of the system.

Unlike the previous examples, the algorithm presented by GAIO does not run a long integration of the model and wait enough time to populate the attractor. Rather, GAIO provides two different ways of computing the transition matrix, namely, computation by *test-points* or computation by *exhaustion*. Using test-points method to compute the transition matrix consists of taking sample points within each box of the discretisation of the phase space and examining where they move after an iteration of the flow. These test points can be randomly chosen so often these points are called Monte Carlo points REF. The exhaustion method works as follows. Consider the boxes A and B , so that we want to estimate the volume of $A \cap T^{-1}(B)$. First, we subdivided a box A into smaller ones of the same size. Second, we test whether the forward image of some of the smaller boxes within A fit into B . If the image does not fit, we reduced the size of the subdivision of A . This idea mimics the exhaustion method that can be found in The Elements.

As an experiment we considered Lorenz' 63 model. First of all we calculate the flow of the system, which is given by the solution of the equation. These experiments are motivated by [14] where similar experiments are performed. The aim is to calculate the response of the system in a finite state Markov chain framework with a transfer operator approach. We note that the procedure we present is different. On one hand, in [14] we observe that a long integration of the equations is done where as here the flow is symbolically approximated using an explicit fourth order Runge-Kutta algorithm as we show below (using MATLAB notation):

```
function X = rk4(v,X,h,n)

% RK4    Fourth order Runge-Kutta algorithm
% performs n steps of the scheme for the vector field v
% using stepsize h on each row of the matrix X
% v maps an (m x d)-matrix to an (m x d)-matrix
```

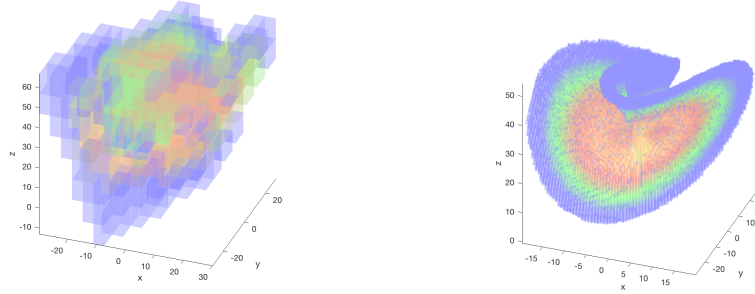


```

for i = 1:n
    k1 = v(X);
    k2 = v(X + h/2*k1);
    k3 = v(X + h/2*k2);
    k4 = v(X + h*k3);
    X = X + h*(k1 + 2*k2 + 2*k3 + k4)/6;
end

```

Secondly, this form of the flow is used to calculate the transition matrix as described in the test-points method, different to that done in [14]. In Figure 5 we observe several outputs of the box covering of the attractor of Lorenz 63 model using GAIO for different resolutions. The command used for the plot is called `boxplot3()`. Although we have not gone into the details, this algorithm also approximates the unstable manifold of the system. It is remarkable that 20 seconds are needed to do a box covering of 33320 microstates.



(a) 342 microstates or boxes.

(b) 33320 microstates or boxes.

Figure 5: Output of GAIO for the box covering of the Lorenz 63 attractor. The red colour indicates the highly populated parts of the attractor.

The existence of a spectral gap in Lorenz 63 model is not apparent from the calculated approximations. For low resolutions, the approximate spectral gap fluctuates to eventually decay in a very slow way (see Figure 6).

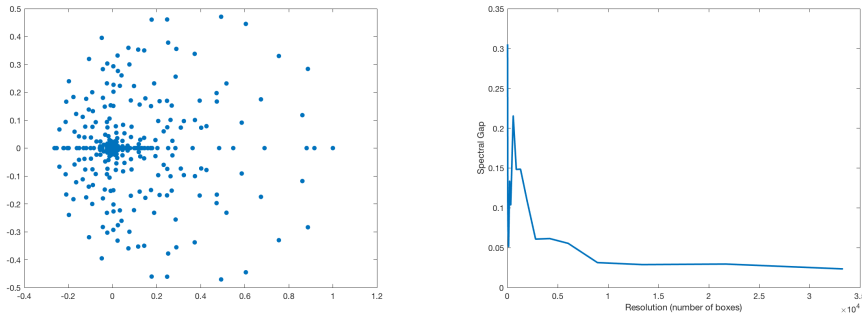


Figure 6: To the left, subset of the complex plane containing the approximate spectrum of the transfer operator of Lorenz 63 for a resolution of 2800 boxes. On the right, the evolution of the spectral gap of the system as a function of the resolution considered.

As commented earlier in the text, the invariant measure of the system is obtained by solving the eigenvalue problem for the eigenvalue 1. Computationally, however, it is not

trivial to solve the eigenvalue problem, especially if one deals with matrices with 33320^2 entries (8.3GB). It is the case that these Markov matrices are sparse and thus we have to manipulate these matrices in sparse mode. MATLAB command `eigs(M,k)` allows us to, iteratively, compute the k largest eigenvalues of the Matrix. In particular for the calculation of the eigenvector associated with the largest eigenvalue (1), we take $k=1$ and $k=2$ when considering the spectral gap.

0.0.4 Lorenz 84

We have also considered Lorenz 84 atmospheric circulation model to test the numerical tools studied so far. Figure 7 shows a reproduction of the experiments done above for Lorenz 84.

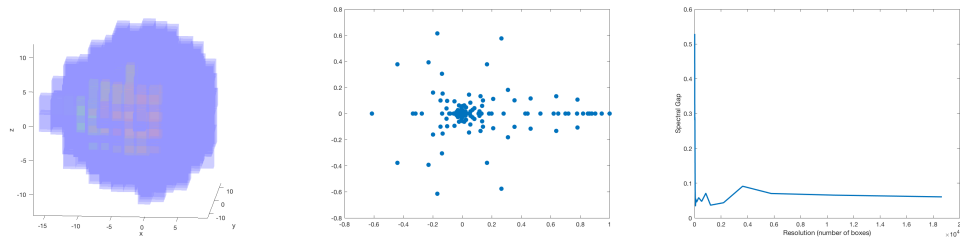


Figure 7: On the left and center figures we see a box covering and the spectrum of the transfer operator of the Lorenz 84 model for a resolution of 256 boxes. The evolution of the spectral gap in Lorenz 84 is shown on the right.

Future Work

The theory concerning Markov operators and their relevance in response theory has to be studied in the next stage of the research project. The spectral properties of the Markov operators describing the evolution of densities in a system is far from trivial and they can change depending on the system we are dealing with. Also, the well-posedness of response theory for certain dynamical system is an open problem. We shall carry on constructing a background in this topic by reading and understanding the results and theory in [11], [6] and [1].

Another target for this project is to become more familiar with the statistical mechanics formulation of response theory. The review article [17] contains the basic formulas and references to construct response theory for infinitesimal and finite perturbations. The overlap between statistical mechanics and dynamical systems is clear today but perhaps an insight to this overlap could be enhanced by getting used to the concepts introduced by D. Ruelle in [19].

The software GAIO uses a set of algorithms that are efficient but not obvious. A deeper understanding of GAIO, particularly of the **Tree** MATLAB class, is needed to be able to extract more dynamical information. Using this package, we will continue to reproduce the results in [14] and [20] and try to calculate the nonlinear terms in the response operator mentioned, also for the observables x^2 , y^2 , z^2 and z . Moreover, we shall move on to testing this approach to more classical models such as Lorenz 84 atmospheric circulation model.

If one produces a very fine approximation of the transfer operator, one has to deal with very large sparse matrices. Iterative methods can be used to compute the largest eigenvalues of such matrices, in particular, the second value λ_2 is the one of physical meaning. Knowing λ_2 allows us to quantify the rate of decay of correlations in the system and to rate the mixing rate. Based on the explicit formulas for λ_2 in [3], it will be an interesting problem to study the behaviour of λ_2 when perturbations are introduced. Generally, the Markov matrices obtain with the approximation of the transfer operator are highly non-normal. Meaning that there can be a severe delay for the measure of the system to be invariant. This delay has to be understood as a transient growth in the norm of the successive powers of the Matrix \mathcal{M} . In [21] we can find a full discussion on this topic that can be applied to our project.

Calculating the response is after all quantifying the *distance* between the unperturbed and the perturbed probability measures. Of course it is not trivial to choose a distance in spaces of measures so it has been recently proposed to use the Wasserstein distance VISSIOLUC. In the next stages of the research, we shall study the properties of this distance and how to implement it. At the moment we have code to compute the distance of combinations of Dirac distributions.

In the context of climate science we will study the ideas developed in [15] in order to link and apply the formalism of response theory. Further, the transfer operators (in general, Markov models) are also a technique used to identify invariant and quasi-invariant sets. This has a wide scope of application when it comes to finding coherent oceanic structures as suggested in LETTER, where they use a data-based construction of the transfer operator. Investigation the resonances in the operator \mathbf{L} in equation (3) can be used to explain low-frequency variability in climate models. In [2] we find a discussion of this method and an application to explain low-frequency variability in the Souther Oscillation.

So far, the research has been devoted to getting familiar with Markov modelling in dynamical systems. Ranging from theoretical environments to numerical approximations, we have studied the basic definitions concerning the functional analytical techniques and

implemented the elementary numerical method in classical models. In the next stage of the research we shall get a deeper insight on the mathematical tools to eventually understand their implications in climate modelling.

Bibliography

- [1] V. Baladi, *Positive Transfer Operators and Decay of Correlations*. Advanced Series in Nonlinear Dynamics, 2000.
- [2] M. D. Chekroun, J. D. Neelin, D. Kondrashov, J. C. McWilliams, M. Ghil, Rough Parameter Dependence and the Role of Ruelle-Pollicot Resonances, *PNAS*, Vol: 111(5), 1684–1690, 2014.
- [3] R. L. Dobrushin, Theory of Probability and its Applications, *Theory of Probability and its Applications*, Vol: 1(1), 65–80, 1956
- [4] M. Dellnitz, G. Froylan, O. Junge, *The Algorithms Behind GAIO-Set Oriented Numerical Methods for Dynamical Systems* in: *Ergodic Theory, Analysis and Efficient Simulation of Dynamical Systems*, Springer, 2001.
- [5] R. Kubo, Statistical-mechanical Theory of Irreversible Processes. I. General Theory and simple Applications to Magnetic and Conduction Problems, *J. Phys. Soc. Jpn.*, Vol: 12, 570–586, 1957.
- [6] M. Hairer, A. J. Majda, A Simple Framework to Justify Response Theory, *Nonlinearity*, Vol: 23, 909–922, 2010.
- [7] M. Hénon, A Two Dimensional Map with a Strange Attractor. *Comm. Math. Phys.*, 50:69–77, 1976.
- [8] G. Keller, C. Liverani, Stability of the Spectrum for Transfer Operators, *Annali della Scuola Normale Superiore di Pisa*, Vol: 28(1), 141–152, 1999.
- [9] A. Lasota, M. C. Mackey, *Chaos, Fractals, and Noise Stochastic Aspects of Dynamics*, Springer-Verlag, 1991.
- [10] G. Lacorata, A. Vulpiani, Fluctuation-Response Relation and Modelling in Systems with Fast and Slow Dynamics, *Nonlinear Processes in Geophysics*, Vol: 14, 681–694, 2007.
- [11] G. Keller, C. Liverani, Stability of the Spectrum for Transfer Operators, *Annali della Scuola Normale Superiore di Pisa*, Vol: 28, 141–152, 1999.
- [12] E. N. Lorenz, Deterministic Nonperiodic Flow, *Journal of the Atmospheric Sciences*, Vol: 20, 130–141, 1963.
- [13] E. N. Lorenz, Deterministic Nonperiodic Flow, *Tellus*, Vol: 36A, 98–110, 1984.
- [14] V. Lucarini, Response Operators for Markov Processes in a Finite State Space: Radius of Convergence and Link to the Response Theory for Axiom A Systems, *Journal of Statistical Mechanics*, Vol: 162, 312–333, 2016.

- [15] C. E. Leith, Climate Response and Fluctuation Dissipation, *Journal of the Atmospheric Sciences*, Vol: 32, 2022–2026, 1975.
- [16] A. Pazy, *Semigroups of Linear Operators and Applications to Partial Differential Equations*. Applied Mathematical Sciences, Springer-Verlag New York, 1983.
- [17] U. M. B. Marconi, A. Puglisi, L. Rondoni, A. Vulpiani, Fluctuation-Dissipation: Response Theory in Statistical Physics, *Physics Reports*, Vol: 461, 111–195, 2008.
- [18] D. Ruelle, A Review of Linear Response Theory for General Differentiable Dynamical Systems, *Nonlinearity*, Vol: 22, 855–870, 2009.
- [19] D. Ruelle, *Thermodynamic Formalism*. Cambridge Mathematical Library, 2004.
- [20] A. Tantet, V. Lucarini, H. A. Dijkstra, Resonances in a Chaotic Attractor Crisis of the Lorenz Flow, *Journal of Statistical Physics*, Vol: 170, 584–616, 2018.
- [21] N. L. Trefethen, M. Embree, *Spectra and Pseudospectra*. Princeton University Press, 2005.
- [22] G. Boffeta, G. Lacorata, S. Musacchio, A. Vulpiani, Relaxation of Finite Perturbations: Beyond the Fluctuation Response Relation, *Chaos*, Vol: 13(3), 806–811, 2003.