

Mathematical and Physical Ideas for Climate Science

Valerio Lucarini

*Klimacampus, Meteorologisches Institut,
University of Hamburg,
20144 Grindelberg 5, Hamburg,
Germany.*

*Department of Mathematics and Statistics,
University of Reading,
Reading, RG6 6AX,
UK.*

Richard Blender, Salvatore Pascale, Jeroen Wouters

*Klimacampus, Meteorologisches Institut,
University of Hamburg,
20144 Grindelberg 5, Hamburg,
Germany.*

Corentin Herbert

*National Center for Atmospheric Research,
P.O. Box 3000, Boulder, CO, 80307,
USA.*

The climate is an excellent example of a forced, dissipative system dominated by nonlinear processes and featuring non-trivial dynamics of a vast range of spatial and temporal scales. The understanding of the climate's structural and multiscale properties is crucial for the provision of a unifying picture of its dynamics and for the implementation of accurate and efficient numerical models. Many open questions remain when trying to put together such a complex picture. How to describe comprehensively the scale-scale interactions and couplings, and how to construct robust, seamless parametrizations in numerical models? How to study the climatic response to perturbations? How to construct a succinct picture of the climate able to summarize its energy fluxes, the energy pathways, and the entropy budget? How to take into account the fundamental symmetries of the system? There has always been a fruitful mutual exchange of ideas, stimulations, methods between climate science and many sectors of applied mathematics and theoretical physics, as clearly showed by examples such as chaos theory, stochastic dynamical systems, turbulence, time series analysis, partial differential equations, and extreme value theory. In this interdisciplinary review, we would like to point out some recent developments at the intersection between climate science, mathematics, and theoretical physics which may prove extremely fruitful in the direction of constructing a more comprehensive account of climate dynamics. We are guided by our interest in exploring the nexus between climate and concepts such as energy, entropy, symmetry, response, multiscale interactions, and its potential relevance in terms of numerical modeling. We describe the powerful reformulation of fluid dynamics made possible by the adoption of the Nambu formalism, and the possible potential of such theory for the construction of more sophisticated numerical models of the geophysical fluids. Then we focus on the very promising results on the statistical mechanics of quasi-equilibrium geophysical flows in a rotating environment, which are extremely useful in the direction of constructing a robust theory of geophysical macro turbulence. The second half of the review is dedicated instead to ideas and methods suited to approaching directly the non-equilibrium nature of the climate system. First, we give an account of some recent findings showing how to use basic concepts of macroscopic non-equilibrium thermodynamics for characterizing the energy and entropy budgets of the climate systems, with the ensuing protocols for intercomparing climate models and developing methods aimed at studying tipping points. These ideas can also create a link between climate science and the growing sector of astrophysics devoted to the investigation of exoplanetary atmospheres. We conclude our review by focusing on non-equilibrium statistical mechanics, which allows for framing in a unified way problems as different as climate response to forcings of general nature, the effect of altering the boundary conditions or the coupling between geophysical flows, and the derivation of parametrizations for numerical models.

I. INTRODUCTION

The Earth's Climate provides an outstanding example of a high-dimensional forced and dissipative complex

system. The dynamics of such system is chaotic, so that there is only a limited time-horizon for skillful prediction,

and is non-trivial on a vast range of spatial and temporal scales, as a result of the different physical and chemical properties of the various components of the climate system and of their coupling mechanisms (*Peixoto and Oort, 1992*).

Thus, it is extremely challenging to construct satisfactory theories of climate dynamics and it is virtually impossible to develop numerical models able to describe accurately climatic processes over all scales. Typically, different classes of models and different phenomenological theories have been and are still being developed by focusing on specific scales of motion (*Holton, 2004; Vallis, 2006*), and simplified parametrizations are developed for taking into account at least approximately what cannot be directly represented (*Palmer and Williams, 2009*).

As a result of our limited understanding of and ability to represent the dynamics of the climate system, it is hard to predict accurately its response to perturbations, were they changes in the opacity of the atmosphere, in the solar irradiance, in the position of continents, in the orbital parameters, which have been present for our planet during all epochs (*Saltzman, 2001*). The full understanding of slow- and fast-onset climatic extremes, such as drought and flood events, respectively, and the assessment of the processes behind tipping points responsible for the multi stability of the climate system are also far from being accomplished.

Such limitations are extremely relevant for problems of paleoclimatological relevance such as the onset and decay of ice ages or of snowball-conditions, for contingent issues like anthropogenic global warming, as well as in the perspective of developing a comprehensive knowledge on the dynamics and thermodynamics of general planetary atmospheres, which seems a major scientific challenge of the coming years, given the extraordinary development of our abilities to observe exoplanets (*Dvorak, 2008*).

Climate science *at large* has always been extremely active in taking advantage of advances in basic mathematical and physical sciences, and, in turn, in providing stimulations for addressing new fundamental problems. The most prominent cases of such interaction are related to the development of stochastic and chaotic dynamical systems, time series analysis, extreme value theory, and fluid dynamics, among others. At this regard, one must note that the year 2013 has seen a multitude of initiatives all around the world dedicated to the theme *Mathematics of Planet Earth*, and, in this context, themes of climatic relevance have been of outstanding relevance.

In this review we wish to present some recent research lines at the intersection between climate science, physics and mathematics. Such approaches seem extremely promising for advancing, on one side, our ability to understand and model climate dynamics, and represent correctly climate variability and climate response to forcings. On the other side, the topics presented here provide examples of how problems of climatic relevance

may pave the way for new, wide-ranging investigations of more general nature.

Of course, our selection is partial and non-exhaustive. We leave almost entirely out of this review very important topics such as extreme value theory (*Ghil et al., 2011*), multiscale techniques (*Klein, 2010*), adjoint methods and data assimilation (*Wunsch, 2012*), partial differential equations (*Cullen, 2006*), linear and nonlinear stability analysis (*Vallis, 2006*), general circulation of the atmosphere (*Schneider, 2006*), macroturbulence (*Lovejoy and Schertzer, 2013*), networks theory (*Donges et al., 2009*), and many relevant applications of dynamical systems theory to geophysical fluid dynamical problems (*Dijkstra, 2013; Kalnay, 2003*).

Our selection will focus, instead, on the concepts of energy, entropy, symmetry, coupling, fluctuations, and response, and also within this realm, we have to make painful choices given the vastness of the field. We are specifically motivated by the desire of bridging the gap between some extremely relevant results in mathematical physics, statistical mechanics, and theoretical physics, and open problems and issues of climate science, hoping to stimulate further investigations and interdisciplinary activities.

We will first concentrate on the properties of inviscid, unforced geophysical flows. In Sec. II, we provide an overview of a very powerful variational formulation of hydrodynamics based on the formalism introduced by (*Nambu, 1973*) and present its applications in a geophysical context, suggesting how these ideas could lead to new generation of numerical models. In Sec. III, starting from the classical investigation by (*Onsager, 1949*) of the dynamics of point vortices, we will show how to develop a statistical mechanical theory of turbulence for geophysical flows in a rotating environment.

We will then move to the paradigm of out-of-equilibrium systems, *i.e.* we firmly set ourselves in the realm of dissipative chaotic flows. In Sec. IV, taking inspiration from the points of view of (*Prigogine, 1961*) and of (*Lorenz, 1967*), we explore how through classical non-equilibrium thermodynamics one can construct tools for assessing the energy budgets and transport, the efficiency, and the irreversibility of the climate system, thus characterizing its large scale properties, and gather information on tipping points. In Sec. V, we address the non-equilibrium statistical mechanics formulation of climate dynamics, and explore how the formalism of response theory allows for addressing in a rigorous framework the climatic response to perturbations, taking inspiration from the work of (*Ruelle, 1997*). In Sec. VI, we present averaging and homogenization techniques, describe how projector operator methods due to (*Mori, 1965*) and (*Zwanzig, 1961*) provide powerful tools for deriving parametrizations and firm ground to the inclusion of stochastic terms and memory effects, and discuss how response theory can be used to derive similar results.

Finally, in Sec. VII we draw our conclusions and

present some perspectives of future research.

II. BEYOND THE HAMILTONIAN PARADIGM: NAMBU REPRESENTATION OF GEOPHYSICAL FLUID DYNAMICS

A. Introduction

Hamiltonian formalism constitutes the backbone of most physical theories. In the case of a discrete system, the basic idea is to provide a full description of the degrees of freedom by defining a set of canonical variables q and of the related momenta p (q and p being N -dimensional vectors), and by identifying the time evolution to a flow in phase space such that the canonical Hamiltonian system H acts as a stream-function, $\dot{q} = \partial_p H, \dot{p} = -\partial_q H$. $H(q, p)$ corresponds to the energy of the system. The flow is inherently divergence free (*solenoidal*), so that the phase space does not contract nor expands, as implied by the Liouville Theorem. As suggested by Noether's theorem, the presence of symmetries in the system implies the existence of so-called physically conserved quantities X_i , such that $\dot{X}_i = 0$. In a system possessing time invariance the energy is constant, while in a system possessing translational invariance, the total momentum M is also constant. A system can possess many constant of motions, apart from energy, but the Hamiltonian plays a special role as it is the only function of phase space appearing *explicitly* in the definition of the evolution of the system (*Landau and Lifshits, 1996*).

Nambu (1973) presented a generalization of canonical Hamiltonian theory for discrete systems. The dynamical equations are constructed in order to satisfy Liouville's Theorem and are written in terms of two or more conserved quantities. The Nambu approach has been extremely influential in various fields of mathematics and physics and is viable to extension to the case of continuum, so that it can be translated into a field theory. The construction of a Nambu field theory for geophysical fluid dynamics went through two decisive steps. The first was the discovery of a Nambu representation of 2D and 3D incompressible hydrodynamics (*Névir and Blender, 1993*). The second important step was the finding that the Nambu representation can be used to design conservative numerical algorithms in geophysical models, and that classical heuristic methods devised by Arakawa for constructing accurate numerical models actually reflected deep symmetries coming from the Nambu structure of the underlying dynamics of the flow (*Salmon, 2005*).

The physical basis for the relevance of the Nambu theory for describing and simulating conservative geophysical fluid dynamics, i.e. stratified and rotating flows comes from the existence of relevant conservation prin-

ciples other than energy's. The first one is the material conservation of potential vorticity, and the second one is the particle relabeling symmetry. These properties are independent from the particular approximated model of the geophysical flow, and are valid for 2D and 3D hydrodynamics, Rayleigh-Bénard convection, quasi-geostrophy, shallow water model, and extends to the fully baroclinic 3D atmosphere. In other terms, the Nambu representation provides the natural description of geophysical fluid dynamics and is superior to the more traditional approaches based essentially on Navier-Stokes equations, just the action-angle representation of the dynamics of a spring is superior to the simple description provided by the second Newton's law of motion.

B. Hydrodynamics in 2D and 3D

In incompressible hydrodynamics enstrophy (in 2D) and helicity (3D) are known as integral conserved quantities besides energy (*Kuroda, 1991*). These two quantities originate in the particle relabeling symmetry in the Lagrangian description of fluid dynamics. *Névir and Blender (1993)* adapted Nambu's formalism to incompressible nonviscous hydrodynamics by using enstrophy and helicity in the dynamical equations.

1. Two-dimensional hydrodynamics

In two dimensions incompressible hydrodynamics is governed by the vorticity equation

$$\frac{\partial \zeta}{\partial t} = -\mathbf{u} \cdot \nabla \zeta \quad (1)$$

with $\zeta = v_x - u_y$ and $\nabla \cdot \mathbf{u} = 0$. The Hamiltonian is the kinetic energy

$$\mathcal{H} = \frac{1}{2} \int \mathbf{u}^2 dA = -\frac{1}{2} \int \zeta \psi dA \quad (2)$$

where ψ is the stream-function for \mathbf{u} , $\mathbf{u} = \mathbf{k} \times \nabla \psi$ (\mathbf{k} denotes the z-unit vector).

The Hamiltonian \mathcal{H} is a functional of velocity. In general functionals are extensive functions in phase space and defined as maps assigning functions to numbers. In the dynamical equations the functional derivative $\delta \mathcal{H} / \delta \zeta$ is needed which describes the change of the functional \mathcal{H} with respect to a changing dynamic variable ζ . The dependency can be explicitly denoted as $\mathcal{H}[\zeta]$. The functional derivative of a functional $\mathcal{G}[f]$ for a function $f(x)$ is defined for a small variation δf in the linear expansion

$$\mathcal{G}[f + \delta f] = \mathcal{G}[f] + \int \frac{\delta \mathcal{G}}{\delta f(x)} \delta f(x) dx + \dots \quad (3)$$

Throughout this review we assume periodic boundary conditions.

The functional derivative $\delta\mathcal{H}/\delta\zeta$ for (2) is explicitly calculated by

$$\begin{aligned}\delta\mathcal{H} &= \int \nabla\psi \cdot \delta\nabla\psi \, dA \\ &= \int \nabla \cdot (\nabla\delta\psi) \, dA - \int \psi\delta\zeta \, dA\end{aligned}\quad (4)$$

Since the first integral vanishes due to the boundary conditions, we obtain $\delta\mathcal{H}/\delta\zeta = -\psi$.

Based on the material advection of the vorticity (1) any functional of the vorticity is conserved

$$\mathcal{C} = \int f(\zeta) \, dA \quad (5)$$

among these the most well-known is enstrophy

$$\mathcal{E} = \frac{1}{2} \int \zeta^2 \, dA \quad (6)$$

The functional derivative of the enstrophy is simply $\delta\mathcal{E}/\delta\zeta = \zeta$.

The 2D vorticity equation can be expressed in a Nambu form using the enstrophy \mathcal{E}

$$\frac{\partial\zeta}{\partial t} = -\mathcal{J} \left(\frac{\delta\mathcal{E}}{\delta\zeta}, \frac{\delta\mathcal{H}}{\delta\zeta} \right) \quad (7)$$

with the Jacobi operator

$$\mathcal{J}(a, b) = \partial_x a \partial_y b - \partial_y a \partial_x b \quad (8)$$

which is an anti-symmetric bracket for the two arguments. Using the aforementioned functional derivatives the vorticity equation (1) is recovered as

$$\frac{\partial\zeta}{\partial t} = \mathcal{J}(\zeta, \psi) \quad (9)$$

The Nambu form (7) represents a field theoretic extension of the dynamics introduced by Nambu (Nambu, 1973) which uses additional conservation laws in the dynamical equations besides the Hamiltonian.

In the following the relationships between Nambu mechanics and Hamiltonian theory are briefly summarized. The time-evolution of an arbitrary functional of vorticity $\mathcal{F} = \mathcal{F}[\zeta]$ is determined by

$$\begin{aligned}\frac{\partial\mathcal{F}}{\partial t} &= - \int \frac{\delta\mathcal{F}}{\delta\zeta} \mathcal{J} \left(\frac{\delta\mathcal{E}}{\delta\zeta}, \frac{\delta\mathcal{H}}{\delta\zeta} \right) \, dA \\ &= \{\mathcal{F}, \mathcal{E}, \mathcal{H}\}\end{aligned}\quad (10)$$

which defines a Nambu bracket for the three functionals involved. The bracket is anti-symmetric in all arguments, $\{\mathcal{E}, \mathcal{H}, \mathcal{F}\} = -\{\mathcal{H}, \mathcal{E}, \mathcal{F}\}$, etc. In general a bracket is an anti-symmetric map in the space of functions. Using rearrangements of these functionals and partial integration it can be shown that the Nambu bracket is cyclic

$$\{\mathcal{F}, \mathcal{E}, \mathcal{H}\} = \{\mathcal{E}, \mathcal{H}, \mathcal{F}\} = \{\mathcal{H}, \mathcal{F}, \mathcal{E}\} \quad (11)$$

The cyclicity of this bracket is a main ingredient in Salmon's application of Nambu mechanics (Salmon, 2005) to construct conservative numerical codes (see Section II.C.2).

A system is Hamiltonian if its dynamics can be written as

$$\frac{\partial\mathcal{F}}{\partial t} = \{\mathcal{F}, \mathcal{H}\}_P \quad (12)$$

with an antisymmetric Poisson bracket. Additionally the bracket has to satisfy the Jacobi identity (see (Takhajan, 1994) for the extension to Nambu brackets).

The Poisson bracket for 2D hydrodynamics (Salmon, 1988; Shepherd, 1990) is easily obtained from the Nambu bracket if the dependency $\delta\mathcal{E}/\delta\zeta = \zeta$ is evaluated

$$\{\mathcal{F}, \mathcal{H}\}_P = \{\mathcal{F}, \mathcal{E}, \mathcal{H}\} = \int \zeta \mathcal{J}(\mathcal{F}_\zeta, \mathcal{H}_\zeta) \, dA \quad (13)$$

with the short cut \mathcal{H}_ζ for the functional derivative (here cyclicity is used (11)).

The Poisson bracket used in Eulerian hydrodynamics is degenerate leading to the notion noncanonical Hamiltonian mechanics. Degeneracy is equivalent to the existence of a so-called Casimir function $\mathcal{C}[\zeta]$ for which the Poisson bracket vanishes for any function $f[\zeta]$

$$\{\mathcal{C}, f\}_P = 0 \quad (14)$$

Casimir functions are automatically conserved due to $\{\mathcal{C}, \mathcal{H}\}_P = 0$. In 2D hydrodynamics Casimirs are given by integrals of arbitrary functions of the vorticity since this annuls (14). Noncanonical Hamiltonian dynamics has been extensively used to investigate non-dissipative hydrodynamics and applications pertain to nonlinear stability analysis, symmetries, and approximation theory (for reviews see (Salmon, 1988; Shepherd, 1990)).

The relationship (13) demonstrates that noncanonical Hamiltonian mechanics is embedded in Nambu mechanics. The main extension is that in Nambu mechanics two Hamiltonians, the enstrophy and the energy, are used (7), and that the Nambu bracket (10) is nondegenerate and void of Casimir functions.

2. Three-dimensional hydrodynamics

Incompressible inviscid fluid dynamics in 3D is determined by the vorticity equation for $\boldsymbol{\xi} = \nabla \times \mathbf{u}$

$$\frac{\partial\boldsymbol{\xi}}{\partial t} = \boldsymbol{\xi} \cdot \nabla \mathbf{u} - \mathbf{u} \cdot \nabla \boldsymbol{\xi} \quad (15)$$

and $\nabla \cdot \mathbf{u} = 0$, with the velocity \mathbf{u} . Total energy

$$\mathcal{H} = \frac{1}{2} \int \mathbf{u}^2 \, dV = -\frac{1}{2} \int \boldsymbol{\xi} \cdot \mathbf{A} \, dV \quad (16)$$

and helicity

$$h = \frac{1}{2} \int \boldsymbol{\xi} \cdot \mathbf{u} \, dV \quad (17)$$

are conserved. \mathbf{A} is the vector potential, $\mathbf{u} = -\nabla \times \mathbf{A}$, with $\nabla \cdot \mathbf{u} = 0$. The functional derivative of the energy with respect to the vorticity is given by $\delta\mathcal{H}/\delta\boldsymbol{\xi} = -\mathbf{A}$ and for helicity $\delta h/\delta\boldsymbol{\xi} = \mathbf{u}$ (compare the 2D version (4)).

The Nambu form of the vorticity equation is

$$\frac{\partial \boldsymbol{\xi}}{\partial t} = K \left(\frac{\delta h}{\delta \boldsymbol{\xi}}, \frac{\delta H}{\delta \boldsymbol{\xi}} \right) \quad (18)$$

with

$$K(\mathcal{A}, \mathcal{B}) = -\nabla \times [(\nabla \times \mathcal{A}) \times (\nabla \times \mathcal{B})] \quad (19)$$

A functional $\mathcal{F} = \mathcal{F}[\boldsymbol{\xi}]$ evolves according to

$$\begin{aligned} \frac{\partial \mathcal{F}}{\partial t} = & - \int \left(\nabla \times \frac{\delta \mathcal{F}}{\delta \boldsymbol{\xi}} \right) \times \left(\nabla \times \frac{\delta h}{\delta \boldsymbol{\xi}} \right) \\ & \cdot \left(\nabla \times \frac{\delta \mathcal{H}}{\delta \boldsymbol{\xi}} \right) \, dV = \{F, h, H\} \end{aligned} \quad (20)$$

The last equation defines the Nambu bracket for 3D hydrodynamics based on the vorticity equation. Helicity is no longer a hidden conserved quantity but enters the dynamics on the same level as the Hamiltonian.

C. Geophysical fluid dynamics

In this section we summarize Nambu representations of the most important models in geophysical fluid dynamics: the quasi-geostrophic potential vorticity equation (*Névir and Sommer, 2009*), the shallow water model (*Salmon, 2005; Sommer and Névir, 2009*), Rayleigh-Bénard equations for two-dimensional convection (*Bihlo, 2008; Salazar and Kurgansky, 2010*), and the baroclinic stratified atmosphere (*Névir and Sommer, 2009*).

1. Quasi-geostrophic approximation

Quasi-geostrophic dynamics in absence of dissipative processes and of forcings is determined by the material conservation of the quasi-geostrophic potential vorticity

$$\frac{\partial Q}{\partial t} + \frac{1}{f_0} J(\Phi, Q) = 0 \quad (21)$$

where J is the Jacobian (8). Q is the quasi-geostrophic approximation of Ertel's potential vorticity

$$Q = \zeta_g + \frac{f_0}{\sigma_0} \frac{\partial^2 \Phi}{\partial p^2} + f \quad (22)$$

with the geostrophic vorticity $\zeta_g = 1/f_0 \nabla_h^2 \Phi$, geopotential Φ , stability parameter σ_0 , and Coriolis parameter f .

The first conserved integral is the total energy

$$\mathcal{H} = \frac{1}{2} \int \left[\left(\frac{\nabla_h \Phi}{f_0} \right)^2 + \left(\frac{1}{N} \frac{\partial \Phi}{\partial z} \right)^2 \right] dV \quad (23)$$

where the first term is the density of kinetic energy and the second term is the density of potential energy *Holton (2004)*. The second conserved integral is potential enstrophy

$$\mathcal{E} = \frac{1}{2} \int Q^2 dV \quad (24)$$

with the Brunt-Vaisala frequency N . The dynamics is determined by the Nambu bracket

$$\frac{\partial \mathcal{F}}{\partial t} = - \int \frac{\delta \mathcal{F}}{\delta Q} J \left(\frac{\delta \mathcal{E}}{\delta Q}, \frac{\delta \mathcal{H}}{\delta Q} \right) dV = \{\mathcal{F}, \mathcal{E}, \mathcal{H}\} \quad (25)$$

which is identical to (10). The Nambu representation of the quasi-geostrophic potential vorticity equation is

$$\frac{\partial Q}{\partial t} = -J \left(\frac{\delta \mathcal{E}}{\delta Q}, \frac{\delta \mathcal{H}}{\delta Q} \right) \quad (26)$$

Thus, the mathematical structure is analogous to the two-dimensional vorticity equation (10).

2. Shallow water model

The Nambu representation of the shallow water model was derived by *Salmon (2005)*. *Sommer and Névir (2009)* present a numerical simulation of these equations on a spherical grid, and *Névir and Sommer (2009)* published the multilayer shallow water equations. Here the single layer model is summarized (*Sommer and Névir, 2009*). The dynamics can be constructed on the evolution equation for the vorticity for the divergence $\mu = \nabla \cdot \mathbf{v}$

$$\partial_t \zeta = -\nabla \cdot (\zeta_a \mathbf{v}) \quad (27)$$

$$\partial_t \mu = k \cdot \nabla \times (\zeta_a \mathbf{v}) + \nabla^2 (\mathbf{v}^2/2 + gh) \quad (28)$$

The shallow water model possesses two conserved integrals, the total energy, given by the sum of kinetic and potential energy

$$\mathcal{H} = \frac{1}{2} \int (h\mathbf{v}^2 + gh^2) dV \quad (29)$$

and potential enstrophy

$$\mathcal{E} = \frac{1}{2} \int hq^2 dV \quad (30)$$

with the absolute potential vorticity $q = \zeta_a/h$, $\zeta_a = \zeta + f$, and the height of the fluid h .

The dynamics of any functional \mathcal{F} is determined by the sum of three Nambu brackets

$$\partial_t \mathcal{F} = \{\mathcal{F}, \mathcal{H}, \mathcal{E}\}_{\zeta, \zeta, \zeta} + \{\mathcal{F}, \mathcal{H}, \mathcal{E}\}_{\mu, \mu, \zeta} + \{\mathcal{F}, \mathcal{H}, \mathcal{E}\}_{\zeta, \mu, h} \quad (31)$$

Here $\mathcal{F}_\zeta = \delta\mathcal{F}/\delta\zeta$, etc. The first bracket is

$$\{\mathcal{F}, \mathcal{H}, \mathcal{E}\}_{\zeta, \zeta, \zeta} = \int J(F_\zeta, H_\zeta) \mathcal{E}_\zeta dA \quad (32)$$

which is analogous to the 2D Nambu bracket (10). For the other brackets we refer to (*Salmon, 2005; Sommer and Névir, 2009*). *Salmon* (2007) calculated the Nambu brackets based on the velocities instead of vorticity.

3. Rayleigh-Bénard convection

Here the equations for the two-dimensional Rayleigh-Bénard convection are summarized (see (*Bihlo, 2008*), *Salazar and Kurgansky* (2010) studied the three-dimensional problem). The fluid flow is incompressible and obeys the Boussinesq approximation in a nondimensional form

$$\frac{\partial \zeta}{\partial t} + [\psi, \zeta] = \frac{\partial T}{\partial x}, \quad \frac{\partial T}{\partial t} + [\psi, T] = \frac{\partial \psi}{\partial x} \quad (33)$$

where $[a, b] = \partial_x a \partial_z b - \partial_z a \partial_x b$ denotes the Jacobian operator. The equations preserve the Hamiltonian

$$\mathcal{H} = \int \left(\frac{1}{2} (\nabla \psi)^2 - Tz \right) dx dz \quad (34)$$

where, as usual, the term in the integral indicate the density of kinetic and potential energy, respectively, and the Casimir

$$\mathcal{C} = \int \zeta(T - z) dx dz \quad (35)$$

This Casimir is a consequence of Kelvin's circulation theorem. The Nambu form of the coupled equations are explicitly written as

$$\frac{\partial \zeta}{\partial t} = - \left[\frac{\delta \mathcal{C}}{\delta T}, \frac{\delta \mathcal{H}}{\delta \zeta} \right] - \left[\frac{\delta \mathcal{C}}{\delta \zeta}, \frac{\delta \mathcal{H}}{\delta T} \right] = \{\zeta, \mathcal{C}, \mathcal{H}\} \quad (36)$$

$$\frac{\partial T}{\partial t} = \left[\frac{\delta \mathcal{C}}{\delta \zeta}, \frac{\delta \mathcal{H}}{\delta \zeta} \right] = \{T, \mathcal{C}, \mathcal{H}\} \quad (37)$$

with the bracket

$$\begin{aligned} \{\mathcal{F}, \mathcal{G}, \mathcal{H}\} = & - \int \left(\frac{\delta \mathcal{F}}{\delta T} \left[\frac{\delta \mathcal{G}}{\delta \zeta}, \frac{\delta \mathcal{H}}{\delta \zeta} \right] \right. \\ & \left. + \frac{\delta \mathcal{F}}{\delta \zeta} \left[\frac{\delta \mathcal{G}}{\delta T}, \frac{\delta \mathcal{H}}{\delta \zeta} \right] + \frac{\delta \mathcal{F}}{\delta \zeta} \left[\frac{\delta \mathcal{G}}{\delta \zeta}, \frac{\delta \mathcal{H}}{\delta T} \right] \right) dx dz \end{aligned} \quad (38)$$

Note that the Casimir (35), as helicity (17), has no definite sign.

4. Baroclinic atmosphere

Névir and Sommer (2009) published the equations determining the dynamics of a baroclinic atmosphere in Nambu form (denoted as Energy-vorticity theory of ideal fluid mechanics). The Nambu representation encompasses the Eulerian equation of motion in a rotating frame, the continuity equation, and the first law of thermodynamics. The Nambu dynamics uses three brackets for energy helicity, energy-mass, and energy-entropy. Due to its special role in all three brackets the integral of Ertel's potential enstrophy is coined as a super-Casimir.

The Nambu form shows an elegant structure where fundamental processes are combined by additive terms. Incompressible, barotropic or baroclinic atmospheres are associated to additive contributions. Thus approximations are simply attained by the neglect of terms.

The momentum equation, the continuity equation and the first law equation are

$$\partial_t \mathbf{v} = \{\mathbf{v}, h_a, H\}_h + \{\mathbf{v}, M, H\}_m + \{\mathbf{v}, S, H\}_s \quad (39)$$

$$\partial_t \rho = \{\rho, M, H\}_m \quad (40)$$

$$\partial_t \sigma = \{\sigma, S, H\}_s \quad (41)$$

with $\sigma = \rho s$, s being the entropy density.

There are four conservation laws. The first is the total energy

$$\mathcal{H} = \int \left\{ \frac{1}{2} \rho \mathbf{v}^2 + \rho e + \rho \Phi \right\} dV \quad (42)$$

e is the specific internal energy and Φ the potential of the gravitational and the centrifugal force. The absolute helicity is

$$h_a = \int \mathbf{v}_a \cdot \boldsymbol{\xi}_a dV \quad (43)$$

where the absolute velocity is $\mathbf{v}_a = \mathbf{v} + \boldsymbol{\Omega} \times \mathbf{r}$ with angular velocity $\boldsymbol{\Omega}$. Mass and entropy are

$$\mathcal{M} = \int \rho dV, \quad S = \int \rho s dV \quad (44)$$

and potential enstrophy is with the potential vorticity Π

$$\mathcal{E}_\rho = \int \rho \Pi^2 dV, \quad \Pi = \frac{\boldsymbol{\xi}_a \cdot \nabla \theta}{\rho} \quad (45)$$

The three brackets are

$$\{\mathcal{F}, h_a, \mathcal{H}\}_h = - \int \left[\frac{1}{\rho} \frac{\delta \mathcal{F}}{\delta \mathbf{v}} \cdot \left(\frac{\delta h_a}{\delta \mathbf{v}} \times \frac{\delta \mathcal{H}}{\delta \mathbf{v}} \right) \right] dV \quad (46)$$

$$\begin{aligned} \{\mathcal{F}, \mathcal{M}, \mathcal{H}\}_m = & - \int \left[\frac{\delta \mathcal{M}}{\delta \rho} \frac{\delta \mathcal{F}}{\delta \mathbf{v}} \cdot \nabla \frac{\delta \mathcal{H}}{\delta \rho} \right. \\ & \left. + \frac{\delta \mathcal{F}}{\delta \rho} \nabla \cdot \left(\frac{\delta \mathcal{M}}{\delta \rho} \frac{\delta \mathcal{H}}{\delta \mathbf{v}} \right) \right] dV + cyc(\mathcal{F}, \mathcal{M}, \mathcal{H}) \end{aligned} \quad (47)$$

$$\{\mathcal{F}, \mathcal{S}, \mathcal{H}\}_s = - \int \left[\frac{\delta \mathcal{S}}{\delta \rho} \frac{\delta \mathcal{F}}{\delta \mathbf{v}} \cdot \nabla \frac{\delta \mathcal{H}}{\delta \sigma} + \frac{\delta \mathcal{F}}{\delta \sigma} \nabla \cdot \left(\frac{\delta \mathcal{S}}{\delta \rho} \frac{\delta \mathcal{H}}{\delta \mathbf{v}} \right) \right] dV + cyc(\mathcal{F}, \mathcal{M}, \mathcal{H}) \quad (48)$$

For a barotropic flow, the first law of thermodynamics and therefore the energy-entropy bracket are omitted. The energy-entropy bracket has to be removed in the Eulerian equation of motion, leading to the energy-vorticity representation of a compressible barotropic fluid. Note the different brackets for velocity (46) and vorticity (20) in 3D hydrodynamics.

D. Conservative algorithms and numerical models

Salmon (2005, 2007) recognized that the existence of a Nambu bracket with two conserved integrals allows the design of conservative numerical algorithms. The single necessary ingredient is that the discrete form of the Nambu bracket preserves antisymmetry. For the barotropic vorticity equation the Arakawa Jacobian could be retrieved by equally weighting the cyclic permutations of the Nambu bracket. The approach is applicable to any kind of discretization, e.g. for finite differences, finite volumes, or spectral models. Furthermore, arbitrary approximations of the conservation laws are possible. The approach is extremely useful in GFD turbulence simulations because these flows are characterized by the existence of conservation laws besides total energy. In particular, the conservation of enstrophy inhibits spurious accumulation of energy at small scales. *Salmon* (2007) presents the first numerical simulation of a shallow water model by equations derived from Nambu brackets. The simulation is on a square rectangular grid and the design on an unstructured triangular mesh is outlined.

Sommer and Névir (2009) report the first simulation of a shallow water atmosphere using Nambu brackets. The authors use an icosahedric grid (as in the ICON model, ICOSahedric Non-hydrostatic model, of the German Weather Service and the Max Planck Institute for Meteorology, Hamburg). The construction of the algorithm is as follows (*Sommer and Névir*, 2009):

- First the continuous versions of the Nambu-brackets and conservation laws need to be given.
- On the grid the following expressions need to be calculated: functional derivatives, discrete operators (div and curl), discretization of the Jacobian and the Nambu brackets.
- Finally the prognostic equations are obtained by inserting the variables in the brackets. The time stepping is arbitrary ((*Sommer and Névir*, 2009) use a leap-frog with Robert-Asselin filter).

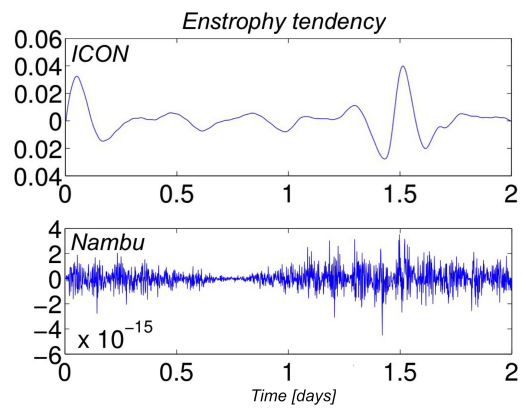


FIG. 1 Enstrophy tendencies in the enstrophy conserving ICON shallow water model and the Nambu model of *Sommer and Névir* (2009) (courtesy of Matthias Sommer, University of München). Note that the tendency in the Nambu model is of the order of the numerical accuracy.

The authors find quasi constant enstrophy and energy compared to a standard numerical design (Fig. 1).

Gassmann and Herzog (2008) suggest a concept for a global numerical simulation of the non-hydrostatic atmosphere using the Nambu representation for the energy-helicity bracket $\{\mathcal{F}, h_a, \mathcal{H}\}$ (*Névir*, 1998). Their suggestion incorporates a careful description of Reynolds averaged subscale processes and budgets. *Gassmann* (2013) describes a global non-hydrostatic dynamical core based on an icosahedral nonhydrostatic model on a hexagonal C-grid. The model conserves mass and energy in a noncanonical Hamiltonian framework. This study notes that there are unsolved numerical problems which occur when the non-hydrostatic compressible equations are in a Nambu bracket form.

E. A phase space view: Lorenz-63 model

(*Nambu*, 1973) introduced his extension of classical Hamiltonian dynamics on the basis of a dynamical system with three degrees of freedom and two conserved quantities. Here we consider the Lorenz-63 model (*Lorenz*, 1963) to present a geometric view of Nambu dynamics in 3D space (for a 10 degree truncation see (*Blender and Lucarini*, 2013)). The conservative parts of the equations are extracted by eliminating the forcing and dissipation terms which violate Liouville's Theorem (*Névir and Blender*, 1994).

In order to distinguish the conservative and dissipative contributions in the Lorenz-63 model a parameter m is introduced which controls the magnitude of the non-

conservative terms ($m = 1$ is the standard case)

$$\dot{x} = \sigma y - \sigma m x \quad (49)$$

$$\dot{y} = r x - x z - m y \quad (50)$$

$$\dot{z} = x y - m b z \quad (51)$$

The equations (49)-(51) with $m = 0$ have two conserved quantities, which can be found by integrating the two equations $dy/dz = (r - z)/y$ and $dz/dy = x/\sigma$

$$H = \frac{y^2}{2} + \frac{z^2}{2} - r z, \quad C = \frac{x^2}{2} - \sigma z \quad (52)$$

H represents available potential energy and C is total energy (see Fig. 2).

Using the two conserved quantities H and C in (52) we can write (49)-(51) in a Nambu representation for $\mathbf{X} = (x, y, z)$, $\nabla = (\partial_x, \partial_y, \partial_z)$

$$\dot{\mathbf{X}} = \nabla C \times \nabla H \quad (53)$$

The system satisfies the Liouville Theorem because the flow $\dot{\mathbf{X}}$ is solenoidal in state space

$$\nabla \cdot \dot{\mathbf{X}} = \nabla \cdot (\nabla C \times \nabla H) = 0 \quad (54)$$

The flow is tangent to both conserved surfaces and parallel to the intersection. Thus, Nambu mechanics provides an illuminating global geometric view of the dynamics. *Roupas* (2012) visualizes the geometry of the conservation laws H and C for different parameters.

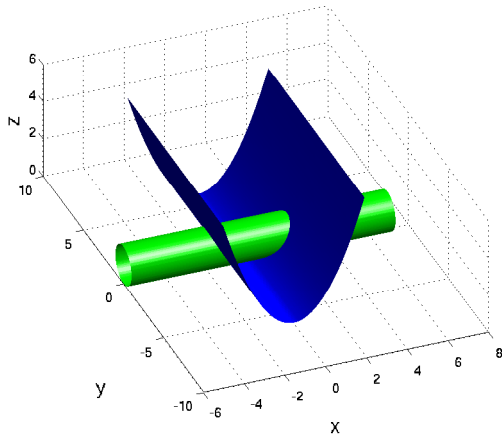


FIG. 2 Conservation laws C and H in the Nambu representation (Eq. 52) of the non-dissipative Lorenz equations (courtesy of Annette Müller, Freie Universität Berlin). Parameters of the model: $r = 1$ and $\sigma = 1$.

F. Perspectives

Like Hamiltonian mechanics, the Nambu approach is a versatile tool for the analysis and simulation of dynamical systems. Here some possible research directions are outlined.

Modular modeling and approximations: In several applications a Nambu representation can be found by adding brackets which conserve a particular Casimir, this is already mentioned by *Nambu* (1973) (see the baroclinic atmosphere (*Névir and Sommer*, 2009) and the classification in (*Salazar and Kurgansky*, 2010)). The dynamics is determined by these 'constitutive' Casimirs (a notion coined in (*Névir and Sommer*, 2009)) which are not conserved in the complete system. Decomposition leads to subsystems where the constitutive Casimirs are conserved. An example is helicity which is constitutive in the baroclinic atmosphere and only conserved in the 3D incompressible flow. The decomposition is directly associated with approximations (*Névir and Sommer*, 2009). Composition allows a process-oriented model design.

Statistical Mechanics: The statistical mechanics of fluids is characterized by the existence of conservation laws besides total energy (*Bouchet and Venaille*, 2012), see also Sect. III in this review. Thus these conservation laws have a two-fold impact: They determine the dynamics in a Nambu bracket and the canonical probability distribution in equilibrium.

Dynamics of Casimirs: Casimir-functions of a conservative system are ideal observables to characterize the dynamics in the presence of forcing and dissipation. *Pelino and Maimone* (2007) and *Gianfelice et al.* (2012) have determined recurrence maps of extremes of energy and a Casimir in a Lorenz-like map to assess predictability and properties of the invariant measure.

III. EQUILIBRIUM STATISTICAL MECHANICS FOR GEOPHYSICAL FLOWS

A. Introduction

The basic idea of equilibrium statistical mechanics is to build a probability measure for the system under consideration, based only on the dynamical invariants. In particular, this is an invariant measure for the original dynamics, provided the Liouville theorem is satisfied (volume in phase space is conserved by the dynamics). This probability measure allows one to compute the statistics of any function of the dynamical variables, which is expected to coincide with the macroscopic behavior of the system, without knowing the details of the microscopic dynamics. This approach, initiated at the end of the 19th century by Boltzmann and Gibbs, has proven very fruitful in classical and quantum mechanics all along the 20th century. However, most of the standard applications of equilibrium statistical mechanics deal with dynamics on a finite dimensional phase space (e.g. finite number of molecules for ideal gas, or finite number of spins for ferromagnetism models), with a finite number of dynamical invariants. The equations describing the dynamics of geophysical flows violate both these con-

straints. Several solutions have thus been proposed: they are reviewed briefly in the next sections, going from the main fundamental ideas¹ to selected geophysical applications². The predictions of the theories take the form of equilibrium states, that is to say the large-scale organization of the flow, and equilibrium spectra for conserved quantities. Equilibrium states include a vast collection of coherent structures, which are indeed observed in nature and numerical experiments. Equilibrium spectra reveal the dominant directions of invariant quantities transfers across the scales of motion. In both cases, the equilibrium methods indicate the natural tendency of the nonlinear evolution. In practice, the system may never reach these equilibrium features, either because of non-ergodicity, or because it is subjected to forcing and dissipation which are not accounted for in this approach. It is worthy of note that, in spite of this, the equilibrium approach still yields useful results to understand the out-of-equilibrium system. Note that the response theory applied to equilibrium states, as first suggested by (*Kubo*, 1957), provides a connection with the non-equilibrium approach, which constitutes a first step to understand departures from equilibrium conditions.

In section III.B, we give a brief account of the point vortex approach introduced by Onsager. Then we discuss the geophysical ramifications of the pioneer work by Kraichnan on Galerkin truncated inviscid flows (section III.C), before introducing the theory developed by Miller, Robert and Sommeria, which treats continuous flows and treats all the invariants (section III.D).

B. Point vortices

1. Negative temperature states and clustering of vortices

Onsager was the first to understand that the coherent structures and persistent circulations that appear ubiquitously in planetary atmospheres and in the Earth's oceans could be explained on statistical grounds (*Onsager*, 1949). His work focused on 2D incompressible, inviscid fluids: $\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P, \nabla \cdot \mathbf{u} = 0$, or equivalently in vorticity form, $\partial_t \omega + \mathbf{u} \cdot \nabla \omega = 0$, with $\omega = \nabla \times \mathbf{u}$. To make the system tractable, he introduced an approximation of the vorticity field in terms of N point vortices with *strength* γ_i and position $\mathbf{r}_i(t)$: $\omega(\mathbf{r}, t) = \sum_{i=1}^N \gamma_i \delta(\mathbf{r}_i(t) - \mathbf{r})$. Introducing the Hamilto-

nian $H = -\sum_{i < j} \gamma_i \gamma_j G(\mathbf{r}_i, \mathbf{r}_j)$, where G is the Green function of the Laplacian, the dynamics reads simply

$$\gamma_i \frac{dx_i}{dt} = \frac{\partial H}{\partial y_i}, \quad \gamma_i \frac{dy_i}{dt} = -\frac{\partial H}{\partial x_i}. \quad (55)$$

This is a canonical Hamiltonian system with a finite number of degrees of freedom, for which the standard methods of statistical mechanics apply directly. In particular, the *microcanonical* probability measure, associating a uniform probability to all the configurations with the same energy, is given by

$$\rho_E(\{\mathbf{r}_i\}_{1 \leq i \leq N}) = \frac{\delta(H(\{\mathbf{r}_i\}_{1 \leq i \leq N}) - E)}{\Omega(E)}, \quad (56)$$

where $\Omega(E)$ is the *structure function*, which measures the volume in phase space occupied by configurations with energy E . It is easily proved that, for a bounded domain, and hence a finite volume phase space, this function reaches a maximum for a given value of the energy. Hence, the thermodynamic entropy $S(E) = k_B \ln \Omega(E)$ decreases for a range of energies, and the statistical temperature $1/T = \partial S / \partial E$ becomes negative. Negative temperatures, although counter-intuitive, have since been commonly encountered in the study of systems with long-range interactions (*Dauvois et al.*, 2002), and correspond to self-organized states. Here, the energy increases when two same-sign vortices move closer, while it decreases for opposite signs. When the temperature is negative, the entropy increases when energy increases, and there is no energy-entropy competition, which results in the appearance of ordered states. Hence, equilibrium states exhibiting clusters of same-sign vortices are expected. This behavior has been confirmed by numerical simulations with up to $N = 6724$ point vortices: see Fig. 3.

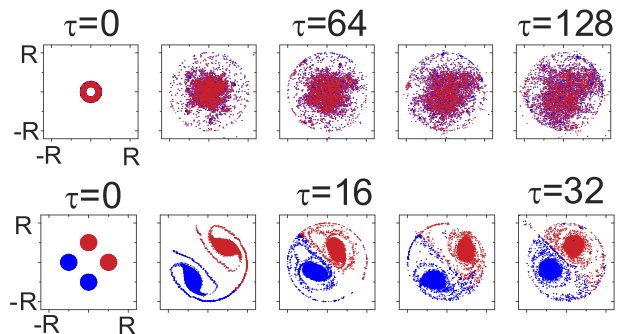


FIG. 3 Time evolution for a numerical simulation of two-sign point vortices, for positive temperatures (upper panel) and negative temperatures (lower panel) (*Yatsuyanagi et al.*, 2005). For negative temperatures, we observe the clustering of same-sign vortices.

¹ Equilibrium statistical mechanics theories for geophysical fluids have also led to progress in statistical mechanics itself, through the theoretical issues of ensemble equivalence, invariant measures, ergodicity,... Due to length constraints, these theoretical developments are not reviewed here.

² Although there are also interesting applications in magnetohydrodynamics, potentially relevant for astrophysical flows, this topic is left aside in the present review.

2. Mean-field equation

The above argument is qualitative; to characterize the coherent structures which are expected to emerge from the clustering of same-sign vortices, we introduce the *mean field* probability density for vorticity: $\rho(\sigma, \mathbf{r}, t) = (1/N) \sum_j \delta(\sigma - \gamma_j) \delta(\mathbf{r} - \mathbf{r}_j(t))$. The probability density for a vortex with strength γ_i to be found at point \mathbf{r} at time t is just $\rho_i(\mathbf{r}, t) = \rho(\gamma_i, \mathbf{r}, t)/n_{\gamma_i}$, where the normalization factor $n_{\gamma} = \sum_j \delta_{\gamma_j \gamma}$ is needed so that $\sum_i \int \rho_i(\mathbf{r}, t) d\mathbf{r} = 1$. We define a *coarse grained* vorticity field $\bar{\omega}(\mathbf{r}, t) = \int \sigma \rho(\sigma, \mathbf{r}, t) d\sigma = \sum_i \gamma_i \rho_i(\mathbf{r}, t)$. The mean-field probability density is expected to converge towards its statistical equilibrium: the equilibrium distribution maximizes the statistical entropy $\mathcal{S} = - \int \rho(\sigma, \mathbf{r}) \ln \rho(\sigma, \mathbf{r}) d\sigma d\mathbf{r} = - \sum_i \int \rho_i(\mathbf{r}) \ln \rho_i(\mathbf{r}) d\mathbf{r}$. The solution of this variational problem is given by $\rho_i(\mathbf{r}) = e^{-\beta(\gamma_i \bar{\psi}(\mathbf{r}) - \mu_i)} / \mathcal{Z}$ where β and $\beta \mu_i$ are the Lagrange parameters associated with conservation of global energy and normalization of each ρ_i , respectively, and $\bar{\psi} = -\Delta^{-1} \bar{\omega}$ is the coarse-grained stream function, while the normalization factor \mathcal{Z} is called the *partition function*. Averaging over this equilibrium distribution gives the coarse-grained vorticity field, which satisfies the *mean-field equation*:

$$\bar{\omega}(\mathbf{r}) = \frac{1}{\mathcal{Z}} \sum_i \gamma_i e^{-\beta(\gamma_i \bar{\psi}(\mathbf{r}) - \mu_i)}. \quad (57)$$

This is an equation of the form $\omega = F(\psi)$, characteristic of the steady-states of the 2D Euler equations. A well-known particular case is that of N vortices with circulation $1/N$ and N vortices with circulation $-1/N$. In that case, the mean-field equation can be recast as $\omega = A \sinh(\beta \Psi)$, with $\Psi = \psi + (\mu_+ - \mu_-)/2$ (*Montgomery and Joyce, 1974*).

The theory can be generalized in a straightforward manner to quasi-geostrophic (QG) flows (*Miyazaki et al., 2011*). (*DiBattista and Majda, 2001*) have given solutions of the mean-field equation for a two-layer model where the point vortices stand for *hetons*, introduced by (*Hogg and Stommel, 1985*) as a model of individual convective towers in the ocean. They have shown that a background barotropic current (the *barotropic governor*) confines potential vorticity and temperature anomalies, thereby suppressing the baroclinic instability, in accordance with numeric simulations (*Legg and Marshall, 1993*).

C. Galerkin truncated flows

1. 2D Turbulence

Rather than a discretization in physical space, one may consider a finite number of modes in Fourier space, as proposed by (*Lee, 1952*) and (*Kraichnan, 1967*) in the context of the Euler equations. For 2D flows —

for simplicity, we consider here a rectangular geometry with periodic boundary conditions; the case of a spherical geometry can be found in (*Frederiksen and Sawford, 1980*) — writing the vorticity field as a truncated Fourier series $\omega(\mathbf{x}) = \sum_{\mathbf{k}} \hat{\omega}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}}$, the evolution in time of the Fourier coefficients follows an equation of the form $\partial_t \hat{\omega}(\mathbf{k}) = \sum_{\mathbf{p}, \mathbf{q}} A_{\mathbf{k}\mathbf{p}\mathbf{q}} \hat{\omega}(\mathbf{p}) \hat{\omega}(\mathbf{q})$, where the summation is restricted to a finite set of wave vectors $\mathcal{B} = \{\mathbf{k} \in 2\pi/L\mathbb{Z}^3, k_{min} \leq k \leq k_{max}\}$. This dynamics preserves two quadratic quantities: the energy $E = \sum_{\mathbf{k}} |\hat{\omega}(\mathbf{k})|^2 / (2k^2)$ and the enstrophy $\Gamma_2 = \sum_{\mathbf{k}} |\hat{\omega}(\mathbf{k})|^2$. (*Kraichnan, 1967*) suggested to consider the canonical probability distribution for the Galerkin truncated system:

$$\rho(\{\hat{\omega}(\mathbf{k})\}_{\mathbf{k} \in \mathcal{B}}) = \frac{e^{-\beta E - \alpha \Gamma_2}}{\mathcal{Z}}, \quad (58)$$

In particular, the average energy at *absolute equilibrium* is given by

$$\langle E \rangle = - \frac{\partial \ln \mathcal{Z}}{\partial \beta} = \frac{1}{2} \sum_{\mathbf{k} \in \mathcal{B}} \frac{1}{\beta + 2\alpha k^2}, \quad (59)$$

which corresponds to an equipartition spectrum for the general invariant $\beta E + \alpha \Gamma_2$: $E(k) = \pi k / (\beta + 2\alpha k^2)$. Inviscid numerical runs indeed relax to this spectrum (*Basdevant and Sadourny, 1975; Fox and Orszag, 1973*). Note that the Lagrange parameters α and β cannot take arbitrary values; they are constrained by the *realizability* condition — for the Gaussian integral defining \mathcal{Z} to converge. Here, this condition reads: $\beta + 2\alpha k_{min}^2 > 0$ and $\beta + 2\alpha k_{max}^2 > 0$. In particular, when $\alpha > 0$, negative temperatures can be attained. In this regime, which corresponds to $\langle \Gamma_2 \rangle / (2\langle E \rangle)$ small enough (*Kraichnan and Montgomery, 1980*), the energy spectrum is a decreasing function of k . When $\beta \rightarrow -2\alpha k_{min}^2$, a singularity appears at $k \rightarrow k_{min}$, which means that the energy is expected to concentrate in the largest scales. Hence, statistical mechanics for the truncated system predicts that when the enstrophy is small enough compared to the energy, we expect the energy to be transferred to the large scales. (*Kraichnan, 1967*) gives other arguments to support and refine this view; in particular he shows the existence of two inertial ranges, with a constant flux of energy and enstrophy, respectively, with the energy spectrum scaling as $E(k) \sim C \varepsilon^{2/3} k^{-5/3}$ and $E(k) \sim C' \eta^{2/3} k^{-3}$ respectively, where ε and η are the energy and enstrophy fluxes. In particular, the equilibrium energy spectrum at large scales is shallower than the energy inertial range spectrum. Assuming a tendency for the system to relax to equilibrium — although the equilibrium is never attained in the presence of forcing and dissipation — we thus expect the flux of energy to be towards the large scales; a process referred to as the *inverse cascade* of 2D turbulence (see Fig. 4). Similarly, the transfer of enstrophy in the corresponding inertial range should be

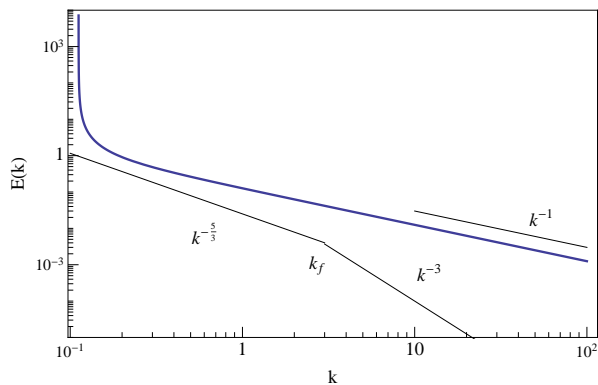


FIG. 4 Energy spectrum (solid blue curve) for 2D turbulence at statistical equilibrium in the negative temperature regime; there is an infrared divergence at k_{min} , corresponding to condensation of energy in the gravest mode. At large k , the equilibrium energy spectrum scales like k^{-1} . We have superimposed on this graph the slopes of the energy and enstrophy inertial ranges, $k^{-5/3}$ and k^{-3} , which build up in the forced case (see text for details).

towards the small scales. The dual cascade scenario has been confirmed both by numerical simulations (*Boffetta, 2007*) and laboratory experiments (*Paret and Tabeling, 1997*).

2. Topographic turbulence

The work of (*Kraichnan, 1967*) was extended to flow over a topography by (*Salmon et al., 1976*) and (*Herring, 1977*). If $H(k)$ is the (prescribed) bottom topography spectrum, the energy spectrum now reads $\langle E(k) \rangle = \pi k / (\beta + 2\alpha k^2) + 2\alpha^2 k^2 / (\beta + 2\alpha k^2)^2 H(k)$. The second term arises because of a non-vanishing mean flow: straightforward computations show that $\langle \hat{\omega}(\mathbf{k}) \rangle = -2\alpha k^2 \hat{h}(\mathbf{k}) / (\beta + 2\alpha k^2)$, so that the second term is the energy spectrum of the mean flow, while the first term stems from the fluctuations. In the absence of topography, the ensemble average vorticity is zero, but in a particular realization, the mean flow will not vanish; the system will spontaneously adopt a choice of phase for each wave vector. Summing over the possible phase choices yields the zero ensemble mean. Note that the mean flow at absolute equilibrium has vorticity proportional to the stream function. This feature has been tested numerically, in connection with the emergence of *Fofonoff* flows (*Griffa and Salmon, 1989*; *Wang and Vallis, 1994*), see Fig. 5. The equilibrium energy spectrum and flow-topography correlation have also been confirmed numerically with very good agreement (*Merryfield and Holloway, 1996*).

3. Quasi-Geostrophic Turbulence

The dynamical equations of QG flow are very similar to the Euler equations, replacing vorticity by potential vorticity. In particular, they conserve similar quadratic invariants, and the theory can be extended in a straightforward manner (*Holloway, 1986*; *Salmon, 1998*). The role of bottom topography has already been investigated in section III.C.2; we will discuss in this section the effect of stratification and beta effect.

Perhaps the simplest framework to consider the role of stratification is the two-layer QG case. As in section III.C.1, a canonical probability distribution can be constructed, taking into account the three invariants: the total energy E and the enstrophies of each layer, Z_1 and Z_2 . The corresponding partition function can be computed, and the spectrum studied in the various regimes, with similar results. In particular, negative temperature states are accessible, which correspond to condensation of the energy on the largest horizontal scales. Maybe more interestingly, although the various forms of energy (kinetic energy K_1, K_2 in each layer and potential energy P) are not individually conserved, we can compute their average value at equilibrium, as (*Salmon et al., 1976*) did. Alternatively, the standard decomposition in terms of the barotropic and baroclinic modes, with their kinetic energies K_T and K_B , can be used. As (*Salmon et al., 1976*) highlighted, the Rossby deformation scale k_D plays an important role. At scales smaller than the deformation scale ($k \gg k_D$), the two layers behave essentially as two independent copies of 2D turbulence; the energy spectrum in each layer is the same as in the 2D case, the correlation at statistical equilibrium is low, and there is about as much energy in the barotropic mode and the baroclinic mode: $\langle K_T(k) \rangle / \langle K_B(k) \rangle \sim 1$. Besides, the potential energy is small compared to the kinetic energy: $\langle P(k) \rangle / \langle K_T(k) \rangle = O(k_D/k)$. At scales larger than the deformation radius ($k \ll k_D$), the system rather behaves as a unique barotropic layer: the amount of energy in the two layers is about the same, but the energy is essentially in the barotropic mode, with negligible energy in the baroclinic mode, and a statistical correlation between the two layers of order 1. This theoretical analysis goes in strong support of the standard picture of two-layer QG turbulence, developed on phenomenological grounds (*Rhines, 1979*; *Salmon, 1978*), see also (*Vallis, 2006, chap. 9*), and is in accordance with numerical simulations (*Rhines, 1976*). These results were extended to an arbitrary number of layers and to continuously stratified flows by (*Merryfield, 1998*). Although the equilibrium mean, vertically integrated stream function remains similar to the two-layer case, the distribution of the statistics on the vertical differs as higher-order moments are considered. The ratio of potential to kinetic energy for instance, can become significantly underestimated, especially in the limit of strong stratification

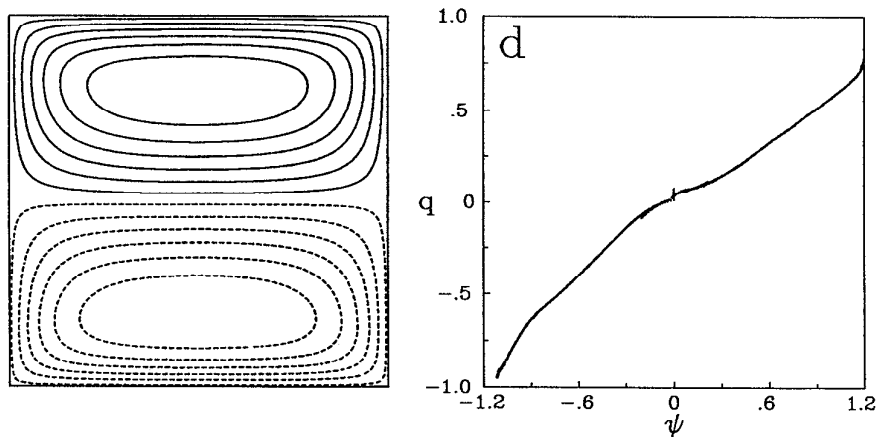


FIG. 5 Convergence towards the statistical equilibrium in inviscid Galerkin-truncated barotropic flow on a β -plane (Wang and Vallis, 1994). Left: Stream function. Right: scatterplot of the q - ψ relation.

($k_D \rightarrow 0$) where the two-layer model does not capture well the possibility that an important fraction of the energy may be trapped near the bottom.

The second dominant effect in geophysical flows, in addition to stratification, is rotation. The Coriolis force introduces a linear term in the equations, which does not affect directly the previous analysis of the nonlinear energy transfers: the conserved quantities remain the same and the statistical theory is easily extended by replacing relative vorticity with absolute vorticity. However, the variation of the Coriolis force with latitude is responsible for the appearance of Rossby waves, which modify the physical interpretation of the predicted cascade of energy. As anticipated by (Rhines, 1975) and verified numerically (e.g Vallis and Maltrud, 1993), the Rossby waves deflect the inverse energy cascade. The ratio of the wave period to the eddy turnover time, $\varepsilon(k) = \tau_W(k)/\tau_{NL}(k)$ gives an estimate of the validity of the above predictions; when $\varepsilon \gg 1$, nonlinear effects dominate, while for $\varepsilon \ll 1$, the waves are much faster than the nonlinear effects and the statistical equilibrium may never be reached. The curve defined by $\varepsilon(k) = 1$ in k -space delimitates the two regimes; it has a dumbbell shape which shows that the waves should prevent access to low wavenumbers along one direction in k -space only. Hence the Rossby waves deflect the cascade and lead to the preferential formation of zonal flows.

4. Beyond balanced motion

Although the motions of the atmosphere and oceans of the Earth are nearly geostrophically balanced, non-balanced motions, like inertia-gravity waves, also play important roles. It is therefore important to understand how energy is exchanged by nonlinear interactions between the slow, balanced motions and the fast, wave motions, and some insight has been gained through equilib-

rium statistical mechanics.

(Errico, 1984) first observed a tendency for unforced inviscid flows described by hydrostatic primitive equations to reach an energy equipartition state, in which the energy in the fast wave modes is comparable to that in the slow balanced modes. The study by (Warn, 1986), in the context of the shallow water equations, essentially confirms that QG flows are not equilibrium states, and that a substantial part of the energy may end up in the fast (surface) wave modes at statistical equilibrium, implying a direct cascade of energy to the small scales. (Bartello, 1995) has obtained analytically the equilibrium energy spectrum for the Boussinesq equations (neglecting the nonlinear part of potential vorticity), in the presence of rotation, confirming the direct cascade of energy. In particular, there is no negative temperature states in this case, due to the presence of the inertia-gravity waves. Studying the resonant triadic interactions, he also discussed the possibility of a wave-vortical mode decoupling, and related the issue of geostrophic adjustment with the existence of an inverse cascade.

Without decoupling assumptions on the dynamics, inverse cascades can be obtained by restricting the computation of the partition function, as done generally when studying metastable states (Penrose and Lebowitz, 1979), to the subset of phase space made of balanced modes. This approach indicates that parity symmetry breaking (Beltrami) flows should display an inverse cascade of energy (Herbert, 2013a). It has also been applied to rotating and/or stratified flows in the Boussinesq approximation (Herbert et al., 2013) to obtain the direction of the energy transfers in anisotropic Fourier space. Combined with an analysis of the deflecting effect of waves similar to the case of Rossby waves (see section III.C.3), this could explain why inverse cascades have been seen in numerical simulations of rotating (e.g. Mininni and Pouquet, 2010) and rotating and stratified (e.g. Marino et al.,

2013) flows, but not in purely stratified flows (e.g. *Waite and Bartello*, 2004).

D. The Robert-Miller-Sommeria theory

The RMS theory bears some resemblance with the point vortices theory; the main difference is that rather than following the (Lagrangian) motion of points with fixed vorticity, the theory is built as the continuous limit of lattice approximations in the Eulerian framework. The rationale behind this choice is, roughly speaking, that although Lagrangian motion is unpredictable, the statistics of the Eulerian flow is (*Robert and Rosier*, 2001).

1. Mean-field theory

Above, we have considered finite-dimensional models conserving two quadratic quantities, the energy and the enstrophy. In fact, the majority of the flows considered above — and in particular 2D and QG flows — conserve an infinite family of invariants, called Casimir invariants: for any function s , $\int s(\omega) d\mathbf{r}$ is conserved. The specific case $s_n(x) = x^n$ corresponds to the moments of the vorticity distribution, $n = 1$ is the circulation and $n = 2$ is the enstrophy, while, $s_\sigma(x) = \delta(x - \sigma)$ yields that the area $\gamma(\sigma)$ where the vorticity takes value σ is conserved. This is due to the absence of a vortex stretching term, in contrast with full 3D flows; here the vorticity (or potential vorticity) patches are stirred in such a way that their area remains conserved, which implies that their boundaries become more and more filamented. The theory developed by (*Miller*, 1990) and (*Robert and Sommeria*, 1991) introduces a coarse-grained vorticity field $\bar{\omega}$, which corresponds to the macroscopic state of the flow. This coarse-grained vorticity field can be predicted based on the invariants using statistical mechanics. To do so, we introduce the probability distribution $\rho(\sigma, \mathbf{r})$ for the vorticity field to take value σ at point \mathbf{r} . The coarse-grained vorticity field is given by $\bar{\omega}(\mathbf{r}) = \int_{-\infty}^{\infty} \rho(\sigma, \mathbf{r}) d\sigma$. The invariants of the system are the energy

$$\mathcal{E}[\rho] = \int_{\mathcal{D}^2} d\mathbf{r} d\mathbf{r}' \int_{\mathbb{R}^2} d\sigma d\sigma' \sigma \sigma' G(\mathbf{r}, \mathbf{r}') \rho(\sigma, \mathbf{r}) \rho(\sigma', \mathbf{r}'), \quad (60)$$

with G the Green function of the Laplacian, and the Casimir invariants

$$\mathcal{G}_n[\rho] = \int_{\mathcal{D}} d\mathbf{r} \int_{\mathbb{R}} d\sigma \sigma^n \rho(\sigma, \mathbf{r}), \quad (61)$$

or equivalently, the vorticity levels

$$\mathcal{D}_\sigma[\rho] = \int_{\mathcal{D}} d\mathbf{r} \rho(\sigma, \mathbf{r}). \quad (62)$$

The idea of the theory is to select the probability distribution ρ which maximizes a *mixing entropy* $\mathcal{S}[\rho] = - \int_{\mathcal{D}} \int_{\mathbb{R}} d\mathbf{r} d\sigma \rho(\sigma, \mathbf{r}) \ln \rho(\sigma, \mathbf{r})$, under the constraints of conservation of the invariants, and point wise normalization $\mathcal{N}[\rho](\mathbf{r}) = \int_{\mathbb{R}} d\sigma \rho(\sigma, \mathbf{r}) = 1$. Hence, we are interested in the variational problem:

$$S(E, \{\Gamma_n\}_{n \in \mathbb{N}}) = \max_{\rho, \mathcal{N}[\rho](\mathbf{r})=1} \{ \mathcal{S}[\rho] \mid \mathcal{E}[\rho] = E, \forall n \in \mathbb{N}, \mathcal{G}_n[\rho] = \Gamma_n \}, \quad (63)$$

or equivalently,

$$S(E, \gamma(\sigma)) = \max_{\rho, \mathcal{N}[\rho](\mathbf{r})=1} \{ \mathcal{S}[\rho] \mid \mathcal{E}[\rho] = E, \forall \sigma \in \mathbb{R}, \mathcal{D}_\sigma[\rho] = \gamma(\sigma) \}. \quad (64)$$

The expression for the mixing entropy \mathcal{S} is justified by the validity of the mean-field theory for long-range interactions (*Bouchet and Venaille*, 2012).

The critical points of the variational problem (64) are simply given by $\delta \mathcal{S} - \int d\mathbf{r} \zeta(\mathbf{r}) \delta \mathcal{N}(\mathbf{r}) - \beta \delta \mathcal{E} - \int d\sigma \alpha(\sigma) \delta \mathcal{D}_\sigma = 0$, where β and $\alpha(\sigma)$ are the Lagrange multiplier associated with the conservation constraints. Easy computations yield the solution

$$\rho(\sigma, \mathbf{r}) = \frac{1}{\mathcal{Z}} e^{-\beta \sigma \bar{\psi}(\mathbf{r}) - \alpha(\sigma)}, \quad (65)$$

so that the coarse-grained vorticity is given by

$$\bar{\omega} = F(\bar{\psi}), \quad \text{with } F(\bar{\psi}) = -\frac{1}{\beta} \frac{\delta \ln \mathcal{Z}}{\delta \bar{\psi}}, \quad (66)$$

and $\mathcal{Z}(\bar{\psi}) = \int_{\mathbb{R}} d\sigma e^{-\beta \sigma \bar{\psi} - \alpha(\sigma)}$. To compute the equilibrium states of the system, one should solve the partial differential equation (66), referred to as the *mean-field equation*, and check afterwards that the obtained critical points are indeed maxima of the constrained variational problem by considering the second derivatives. This will automatically ensure that the equilibrium states are nonlinearly stable (*Chavanis*, 2009).

2. Equilibrium states for 2D and barotropic flows

The mean-field equation (66) is in general difficult to solve; one issue is that the $\bar{\omega} - \bar{\psi}$ relation is in general nonlinear. Most of the analytical solutions have been obtained in the linear case, by decomposing the fields on a basis of eigenfunctions of the Laplacian on the domain \mathcal{D} . This technique was first introduced in a rectangular domain by (*Chavanis and Sommeria*, 1996), who showed that the statistical equilibrium is either a monopole or a dipole, depending on the aspect ratio (Fig. 6).

The same method was extended to the case of barotropic flows, replacing vorticity by potential vorticity. Taking into account the beta effect, Fofonoff flows are

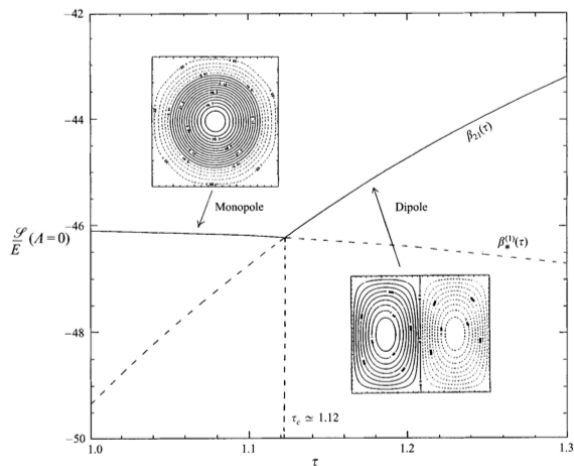


FIG. 6 Maximum entropy states as a function of the aspect ratio for a rectangular domain, in the linear (*strong mixing*) ω - ψ limit (Chavanis and Sommeria, 1996). For $\tau < \tau_c$, the equilibrium is a monopole, while for $\tau > \tau_c$, it is a dipole.

obtained as statistical equilibria in a rectangular basin (Naso et al., 2011; Venaille and Bouchet, 2011a). On a rotating sphere, the equilibria, in the linear limit, can be either solid-body rotations or dipole flows (Herbert et al., 2012a,b). Note that in general, in the linear limit, all the energy is expected to condense into the gravest modes in the equilibrium state (Bouchet and Corvellec, 2010). The effect of the higher-order, fragile Casimir invariants³ is to prevent complete condensation, leading to a wider variety of flow topologies at equilibrium, and to non-linear $\bar{\omega}$ - $\bar{\psi}$ relationships. The condensation can also be arrested due to geometric effects, as in the case of the sphere, for which additional invariants appear (Herbert, 2013b). (Bouchet and Simonnet, 2009) have also considered the role of a small nonlinearity in the $\bar{\omega}$ - $\bar{\psi}$ relationship for a rectangular domain of aspect ratio close to 1, thereby obtaining two topologies for the equilibrium states: dipole and unidirectional flows. Adding a small stochastic forcing generates transitions from one to the other equilibrium.

In the case of the equivalent barotropic model, for which the potential vorticity is given by $q = -\Delta\psi + \psi/R^2 + h$, the Rossby deformation radius R introduces a new length scale. Another limit which is analytically solvable is that of a very small Rossby deformation radius: $R \ll L$, where L is the size of the domain. This limit leads to sharp interfaces separating phases of different free energies, characterized by different, well homogenized potential vorticities (Bouchet and Sommeria,

2002). Strong jets form at the interface between two such homogeneous potential vorticity regions; mid basin eastward jets, such as the Gulf Stream and the Kuroshio, can be interpreted as such statistical equilibria when the beta effect is neglected, but in the presence of beta effect, these solutions become metastable or unstable (Venaille and Bouchet, 2011b). In the jet regions, mesoscale rings form and propagate westward (Chelton et al., 2007). (Venaille and Bouchet, 2011b) have shown that mesoscale rings could also be seen as local equilibrium states in a channel (see Fig. 7).

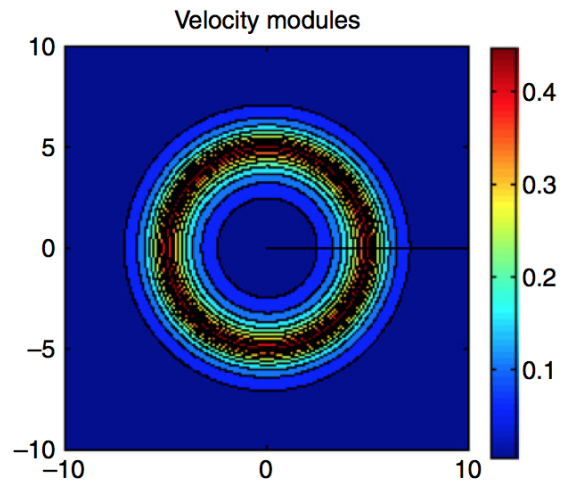


FIG. 7 Modulus of the velocity in the ring statistical equilibrium of the QG model in the limit of small Rossby deformation radius R (Venaille and Bouchet, 2011b). The width of the jet is of order R .

3. Stratified flows

In addition to the 2D and quasi-2D cases mentioned above, the RMS theory has also been applied to stratified fluids (essentially in the quasi-geostrophic regime). (Herbert, 2013c) has obtained and classified the statistical equilibria of the two-layer QG model in the framework of the RMS theory, and updated the discussion of the vertical distribution of energy at statistical equilibrium (see section III.C.3). In the context of continuously stratified flows, (Venaille, 2012) has taken up the thread initiated by (Merryfield, 1998) (see section III.C.3) and shown that bottom-trapped currents are indeed statistical equilibria of the RMS theory. Still in the continuous case, (Venaille et al., 2012) have also studied the vertical distribution of energy at statistical equilibrium, focusing on the tendency to reach barotropic equilibrium states; as also observed in the two-layer model, the constraint of conservation of fine-grained enstrophy prevents complete barotropization. As the beta effect increases, barotropization is facilitated, until we enter a regime dominated by waves.

³ As the fragile invariants cannot be recovered from the predicted coarse-grained field, it was suggested to treat them in a canonical manner (Turkington, 1999). This introduces the conceptual difficulty of defining a potential vorticity reservoir.

E. Subgrid scale parameterization

The equilibrium approach has found other practical applications with parameterization methods. A notable one is the *Neptune effect parameterization*: given the tendency of ideal Galerkin truncated flows to go towards the state of maximum entropy (*Zou and Holloway, 1994*), (*Holloway, 1992*) suggested that instead of the usual subgrid scale parameterizations in ocean models (e.g. eddy viscosity $\nu_*\Delta\mathbf{u}$), which drives the system towards rest, one should use a relaxation towards the statistical equilibrium state \mathbf{u}^* (e.g. of the form $\nu_*\Delta(\mathbf{u} - \mathbf{u}^*)$ for eddy viscosity). This parameterization has been used tested and commented in a number of studies (*Cummins and Holloway, 1994*, e.g.). For more perspective on this type of subgrid-scale parameterizations, the reader is referred to (*Holloway, 2004*) and (*Frederiksen and O’Kane, 2008*).

Along similar lines, (*Kazantsev et al., 1998*) have proposed more generally to treat the subgrid scales so as to maximize the entropy production, inspired by the relaxation equations formulated in the RMS theory (*Chavanis and Sommeria, 1997*). Note also that it has been shown in direct numerical simulations of ideal 3D turbulence that the small scales thermalize progressively, and act as a sort of effective viscosity even in the ideal system, leading to the appearance of transient Kolmogorov scaling laws (*Cichowlas et al., 2005*). This seems to be consistent with the above suggestions for subgrid scale parameterizations.

IV. THERMODYNAMICS OF FORCED AND DISSIPATIVE SYSTEMS

A. Introduction

The atmosphere and the oceans are out-of-equilibrium systems, which exchange irreversibly matter and energy from their surrounding environment and re-export it in a more degraded form at higher entropy. For example, Earth absorbs short-wave radiation (low entropy solar photons at $T_{sun} \approx 6000$ K) which is then re-emitted to space as infrared radiation (high entropy thermal photons at $T_{earth} \approx 255$ K). In addition to that, spatial gradients in chemical concentrations and temperature as well as their associated internal matter and energy fluxes can be established and maintained for long time within nonequilibrium systems (e.g. the temperature contrast between the polar and equatorial regions and the associated large-scale, atmospheric and oceanic circulation). In contrast, closed, isolated systems cannot maintain disequilibrium and evolve towards structureless, homogenous thermodynamical equilibrium, as a result of the second law of thermodynamics (*Prigogine, 1961*).

The basis of the physical theory of climate was established in a seminal paper by (*Lorenz, 1955*), who elu-

cidated how the mechanisms of energy forcing, conversion and dissipation are related to the general circulation of the atmosphere. Oceanic and atmospheric large scale flows result from the conversion of available potential energy - coming from the differential heating due to the inhomogeneity of the absorption of solar radiation - into kinetic energy. through different mechanisms of instability due to the presence of large temperature gradients. The understanding of the fundamentally thermodynamical origin of such dynamical instabilities, as clarified by (*Charney, 1947*) and (*Eady, 1949*), is the other cornerstone of geophysical fluid dynamics. Such instabilities create a negative feedback, as they tend to reduce the temperature gradients they feed upon by favoring the mixing between masses of fluids at different temperatures. Attaining the closure of such a thermodynamical/dynamical problem would mean obtaining a self-consistent theory of climate able to connect instabilities and large scale stabilizing processes on longer spatial and temporal scales.

Furthermore, in a forced and dissipative system like the Earth’s climate, entropy is continuously produced by irreversible processes and at steady state, the entropy production is balanced by a net outgoing flux of entropy at the boundary of the system, in our case, the top of the atmosphere. Therefore, on the average the entropy budget - just like the energy budget - vanishes (*deGroot and Mazur, 1984; Prigogine, 1961*). Besides the dissipation of kinetic energy due to viscous processes, many other irreversible processes such as turbulent diffusion of heat and chemical species, irreversible phase transitions associated to various processes relevant for the hydrological cycle, and chemical reactions relevant for the biogeochemistry of the planet contribute to the total material entropy production (*Goody, 2000; Kleidon, 2009*). The study of the climatic entropy sources (*Fraedrich and Lunkeit, 2008; Goody, 2000; Kleidon, 2009; Kleidon and Lorenz, 2005; Lucarini et al., 2011; Pascale et al., 2011; Pauluis and Held, 2002a,b*) has been revitalized after (*Paltridge, 1975, 1978*) proposed a principle of maximum entropy production (MEPP) as a constraint on the climate system. Although there is still great confusion about MEPP and other nonequilibrium variational principles (for an updated review see *Dewar et al., 2013*), this has led the scientific community to refocus on the importance of a thermodynamical approach - as complementary to the dynamical one - for studying classes of problems like those relevant for nonlinear geophysical flows.

B. Climatic energy budget and energy flows

1. Conservation of energy

A detailed knowledge of the energy flows and their response to perturbations is fundamental for progressing understanding of the climate system. The right closure of the energy budget and an accurate representation of the transport of energy in all forms have to be properly accounted for in any climate model in order to have a good representation of the climate state. The total specific energy of a geophysical fluid is given by the sum of internal, potential, kinetic and latent energy, $e = i + \phi + k + l$ ($e = c_v T + gz + \mathbf{v}^2/2 + Lq$ for the atmosphere and $e = c_0 T + gz + \mathbf{v}^2/2$ for the ocean, standard notation is used). The conservation of energy and mass require that (Peixoto and Oort, 1992):

$$\frac{\partial \rho e}{\partial t} = -\nabla \cdot (\mathbf{J}_h + \mathbf{F}_R + \mathbf{F}_S + \mathbf{F}_L) - \nabla(\tau \cdot \mathbf{v}) \quad (67)$$

where ρ is the density; t is time; \mathbf{v} is the velocity vector; \mathbf{F}_R , \mathbf{F}_S , and \mathbf{F}_L are the vectors of the radiative, turbulent sensible, and turbulent latent heat fluxes, respectively; p is the pressure; and τ is the stress tensor and the total enthalpy transport $\mathbf{J}_h = (\rho e + p)\mathbf{v} = \rho h\mathbf{v}$ has been introduced. By expressing Eq. (67) in spherical coordinates (r, λ, φ) and assuming the usual thin shell approximation $r = R + z$, $z/R \ll 1$, where R is the Earth's radius and z is the vertical coordinate of the fluid, it can be shown that:

$$[\dot{E}] = -\frac{1}{R \cos \varphi} \frac{\partial T_T}{\partial \varphi} + [F_R]_{toa} \quad (68)$$

in which $[E](\varphi, t) \equiv \int E(\lambda, \varphi, t) d\lambda$ and the meridional enthalpy transport has been defined as:

$$T_T(\varphi, t) \equiv \iint J_{h\varphi}(\varphi, \lambda, z, t) R \cos \varphi dz d\lambda. \quad (69)$$

Equation (68) relates the rate of change of the vertically and zonally integrated total energy to the divergence of the meridional transport by the atmosphere and oceans and the zonally integrated radiative budget at the top-of-the-atmosphere. Integrating along φ ($\{X\} = \int X d\varphi$), the expression for the time derivative of the net global energy balance is straightforwardly derived:

$$\{[F_R]_{toa}\} = \{[\dot{E}]\}. \quad (70)$$

Similar relationships can be written for the atmosphere, ocean and land provided that energy fluxes of sensible, latent heat as well as radiative fluxes are taken into account at the surface (Lucarini and Ragone, 2011).

Under steady state conditions, the long term average $\bar{\dot{E}} = 0$ because otherwise, trends would be present.

Therefore from equation (70) the stationarity condition implies that

$$\overline{\{[F_R]_{toa}\}} = 0. \quad (71)$$

Equation (71) is a particular case of a general property of forced dissipative systems that, under generic boundary conditions, realize steady states obeying zero sum properties for energy fluxes on the average (Prigogine, 1961). A physically consistent climate model therefore should feature a vanishing net energy balance when statistical stationarity is eventually obtained. Lucarini and Ragone (2011) analyzed the behavior of more than twenty atmosphere-ocean coupled climate models (PCMDI/CMIP3 intercomparison project, <http://www-pcmdi.llnl.gov/>) under steady state conditions (preindustrial scenario) and found that models' energy balances are wildly different with global balances spanning between -0.2 and 2 W m^{-2} , with a few ones featuring imbalances larger than 3 W m^{-2} . We have analyzed similar budgets for the last generation of climate models (CMIP5 intercomparison project, Taylor et al. (2012)) and have not found a significant improvement (Fig. 8). Spurious energy biases may be associated with non-conservation of water in the atmospheric branch of the hydrological cycle (Liepert and Lo, 2013) and in the water surface fluxes (Hasson et al., 2013; Lucarini et al., 2008), with the fact that dissipated kinetic energy is not re-injected in the system as thermal energy (Becker, 2003), as well as with nonconservative numerical schemes (Gassmann, 2013).

2. Meridional enthalpy transport

The meridional distribution of the radiative fields at the top-of-the-atmosphere poses a strong constraint on the meridional general circulation (Stone, 1978). As clear from equation (68), the stationarity condition (71) leads to the following indirect relationship for T_T :

$$\overline{T_T}(\varphi) = -2\pi \int_{\varphi}^{\pi/2} R^2 \cos \varphi' \overline{(F_R)_{toa}}(\varphi'). \quad (72)$$

In other terms, the flux T_T results from the fact that low-latitude zones feature a positive imbalance between the net input of solar radiation – determined by planetary albedo, i.e. clouds (Donohoe and Battisti, 2012) – and the output of longwave radiation, while the high latitudes feature a negative imbalance. Atmospheric and oceanic circulations act as responses needed to equilibrate such an imbalance.

The climatic meridional enthalpy transport $T_T(\varphi)$ – and its atmospheric and oceanic components, T_A and T_O – is a fundamental measure of nonequilibrium and provides a concise picture of the processes by which the climatic fluid reduces the temperature difference between

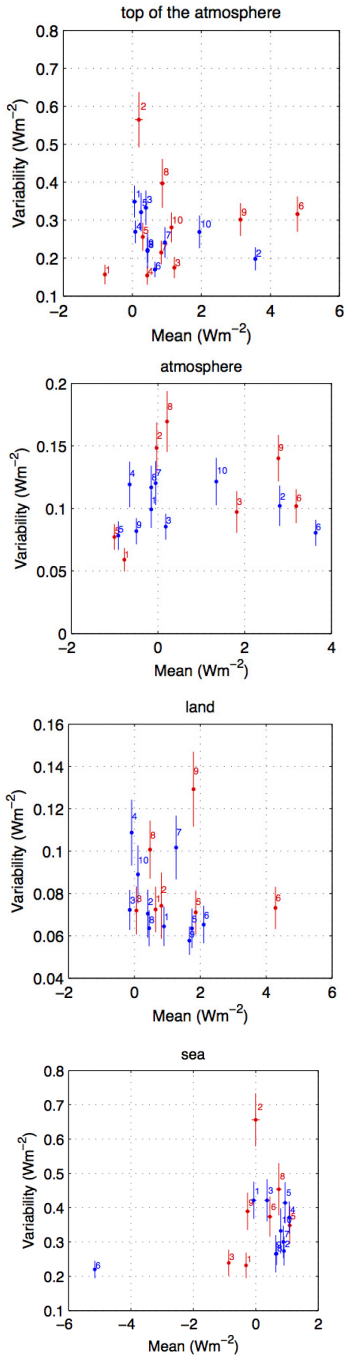


FIG. 8 Mean and standard deviation of globally averaged top-of-the-atmosphere radiative budget (top), atmosphere energy budget (top-middle), ocean (bottom-middle) and land energy budget (bottom) for inter-comparable CMIP3 (red) and CMIP5 (blue) climate models control simulations.

the low and high latitude regions with respect to what imposed by the radiativ-convective equilibrium picture. *Stone* (1978) showed that T_T depends essentially on the mean planetary albedo and on the equator-to-pole contrast of the incoming solar forcing, while being mostly independent from dynamical details of atmospheric and

oceanic circulations. As emphasized by *Enderton and Marshall* (2009), if one assumes drastic changes in the meridional distributions of planetary albedo differences emerge with respect to *Stone's* theory. A comprehensive thermodynamic theory of the climate system able to predict the peak location and strength of the meridional transport, the partition between atmosphere and ocean (*Rose and Ferreira*, 2013) and to accommodate the variety of processes contributing to it, is still missing.

Besides theoretical difficulties, observational estimations of T_T , T_A and T_O also poses non-trivial challenges. For simplicity, we here refer to T_T . There is still not an accurate estimate of such a fundamental quantity for testing the output of climate models, despite the efforts of several authors (*Fasullo and Trenberth*, 2008; *Mayer and Haimberger*, 2012; *Trenberth and Caron*, 2001; *Trenberth and Fasullo*, 2010; *Wunsch*, 2005). The precision of the estimates relies on the knowledge of the *boundary fluxes* \mathbf{F}_R , \mathbf{F}_S , and \mathbf{F}_L and on the reanalysis datasets. *Wunsch* (2005), by using measurements of the radiative fluxes at the top of the atmosphere and previous estimates of the oceanic enthalpy transport, gave a range of values of 3.0 – 5.2 PW (1 PW = 10^{15} W) for the maximum in the Northern Hemisphere (NH) and 4.0 – 6.7 PW for the maximum in the Southern Hemisphere (SH). *Trenberth and Fasullo* (2010), by combining measurements of top-of-the-atmosphere radiative fields with different reanalyses and ocean datasets, found the range to be 4.7 – 5.1 PW for the SH maximum and 4.6 – 5.6 PW for NH. *Mayer and Haimberger* (2012), using two reanalysis datasets (ERA-40 and the more recent ECMWF reanalysis ERA-Interim), constrained the two peaks in narrower confidence intervals: 5.1 – 5.6 PW in the SH (4.4 – 4.9 PW in the NH) for the ERA-40 data and 5.1 – 5.6 PW in the SH (4.4 – 4.9 PW in the NH) for the ERA-Interim data. Unfortunately reanalysis datasets are affected by mass and energy conservation (e.g. $+1.2 \text{ W m}^{-2}$ at the top-of-the-atmosphere and $+6.8 \text{ W m}^{-2}$ over oceans in ERA-Interim, (*Mayer and Haimberger*, 2012)) problems that may potentially bias the transport estimates. Furthermore, these estimates are dependent on the analysis method and the model used – *Trenberth and Caron* (2001), using other reanalysis dataset (NCEP), found a value of the maxima 0.6 PW larger in the NH than those found with the ECMWF reanalysis.

The use of numerical climate model does not help to reduce such uncertainties *Lucarini and Ragone* (2011) analyzed a large dataset of coupled climate models (PCMDI/CMIP3, <http://www.pcmdi.llnl.gov/>) and found a large spread in the meridional enthalpy transports peaks with discrepancies of the order of 15-20 % around a typical value of about 5.5 PW. State-of-the-art climate models (CMIP5 intercomparison project, *Taylor et al.* (2012)) show little improvement in terms of mutual agreement (Fig. 9). *Donohoe and Battisti* (2012) attributed such a large spread in T_T to intermodel dif-

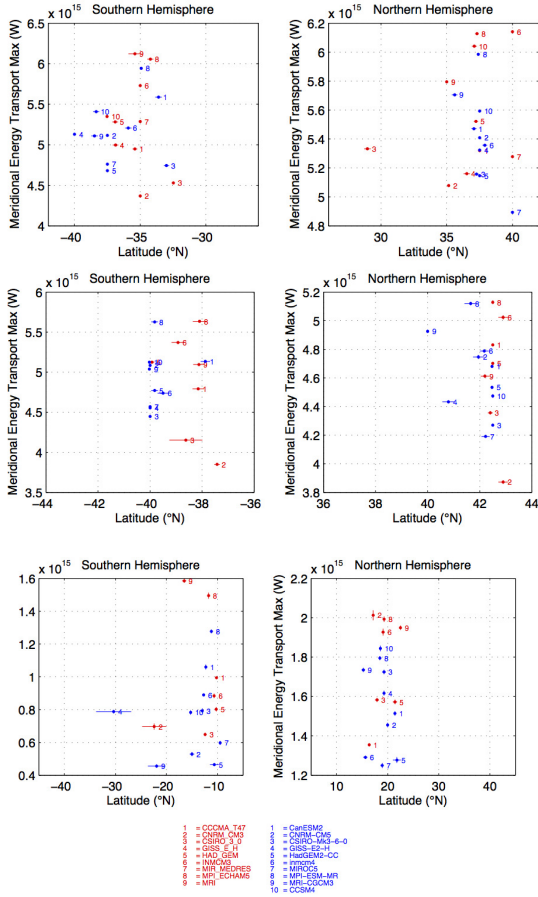


FIG. 9 Value and position of the peak of the poleward meridional enthalpy transport in the pre-industrial scenario for the whole climate (top), atmosphere (middle) and ocean (bottom) for the some of the CMIP3 (red) and CMIP5 (blue) general circulation models.

ferences in the meridional contrast of absorbed solar radiation, which, in turn, is mainly due to the inter-model difference in the shortwave optical properties of the atmosphere (cloud distribution). Figure 9 also shows that, while the disagreement among models for the peak of the atmospheric transport is comparable to that for the peak of the total transport, enormous differences emerge when comparing oceanic transports.

Interesting information emerge when looking at the position of the peaks of the transport. *Stone (1978)* predicts that the position of the maximum of T_T is well constrained by the geometry of the system and weakly dependent of longitudinal homogeneities, and, accordingly in Fig. 9 both CMIP3 and CMIP5 models feature small spread in the position of the peak of T_T , with minute differences between the two hemispheres, except one outlier. Similarly, the spread among models is small with respect to the position of the peak of T_A in both hemispheres and of T_O in the Northern Hemispheres, while a larger uncertainty exists in the position of the peak of T_O in the Southern Hemisphere.

C. The maintenance of thermodynamical disequilibrium

The basic understanding of the maintenance of the atmospheric general circulation was achieved nearly sixty years ago by E. N. Lorenz (*Lorenz, 1955*) through the concepts of available potential energy and atmospheric energy cycle. The concept of available potential energy, first introduced by *Margules (1905)* to study storms, is defined as $A = \int c_p(T - T_r)dV$, where T_r is the temperature field of the reference state, obtained by an isentropic redistribution of the atmospheric mass so that the isentropic surfaces become horizontal and the mass between the two isentropes remains the same. By its own definition, this state minimizes the total potential energy at constant entropy. Such a definition is somewhat arbitrary and different definitions lead to different formulations of atmospheric energetics. For example, the choice of a reference state maximizing entropy at constant energy (*Dutton, 1973*) leads in a natural way to the concept of exergy⁴, common in heat engines theory (*Rant, 1956*). A review on the various theories of available energetics and their link to exergy, is given by (*Tailleux, 2013*). In-depth literature on the Lorenz’s energetics theory can be found in (*Lorenz, 1967*) and (*Peixoto and Oort, 1992*). Here a succinct review of the global thermodynamical properties of the atmosphere is presented and the main implications of the first and second law of thermodynamics are analyzed.

The total energy budget of the atmosphere can be written as $E = P + K$, where $K = (1/2) \int \mathbf{v}^2 \rho dV$ represents the total kinetic energy and $P = \int (c_p T + Lq) \rho dV$ the total potential energy⁵ and V is the atmospheric domain. It can be shown (*Peixoto and Oort, 1992*) that:

$$\dot{P} = -W(P, K) + \dot{\Psi} + D, \quad (73)$$

$$\dot{K} = -D + W(P, K), \quad (74)$$

in which $D = \int \rho \epsilon^2 dV > 0$ is the dissipation of kinetic energy due to friction, $W(P, K) = - \int \mathbf{v} \cdot \nabla p p dV$ is the potential-to-kinetic energy conversion rate and $\dot{\Psi} = \int \dot{q}_{nf} dV$ is the non-frictional diabatic heating due to the convergence of turbulent sensible heat fluxes, condensation/evaporation, and convergence of radiative fluxes. The conversion term W can be interpreted as the the instantaneous work performed by the system. In this respect, equation (73) represents the statement of the first law of thermodynamics for the atmosphere. Equations

⁴ Exergy is the part of the internal energy measuring the departure of the system from its thermodynamic and mechanical equilibrium, that is a state of maximum entropy at constant energy.

⁵ The total potential energy is locally defined as $c_v T + gz + Lq$. However under the hydrostatic approximation it is straightforward to show that $\int (c_v T + gz) \rho dz = \int c_p T \rho dz$ (see e.g. *Lorenz, 1967*).

(73)-(74) imply that $\dot{E} = \dot{P} + \dot{K} = \dot{\Psi}$ and therefore the frictional heating D does not increase the total energy since it is just an internal conversion between kinetic and potential energy. The terms involved in eqs. (73)-(74) are schematically shown in Fig. 10. Stationarity implies that $\bar{P} = \bar{K} = 0$ and therefore $\bar{D} = \bar{W}$. A third independent measure of the strength of the Lorenz's energy cycle not implicit in equations (73)-(74) is the generation of available potential energy, $G = \int \dot{q}_{nf}(1 - T/T_r)dV$ in which T_r is the temperature field of the reference state and, for a steady state, $\bar{G} = \bar{W} = \bar{D}$. Lorenz (1955) showed that $\bar{G} \approx \int \gamma T' \widetilde{q'_{nf}} \rho dz$, which emphasizes the dependence of G on the gross static stability $\gamma = -(R\theta/c_p p T)(\partial\theta/\partial p)$ (vertical structure of the atmosphere) and on the covariance of temperature and heating on pressure levels $T' \widetilde{q'_{nf}}$ (horizontal structure of the atmosphere).

The strength of the Lorenz energy cycle is a fundamental nonequilibrium property of the atmosphere, which just as the meridional enthalpy transport (Sect. IV.B.2), is known with large uncertainty. Reanalysis (with all associated problems, see Sect. IV.B.2) constrain \bar{D} in the range $1.5 - 2.9 \text{ W m}^{-2}$ (Li *et al.*, 2008). On the other hand, general circulation models feature values of \bar{D} from 2 to 3.5 W m^{-2} (Marques *et al.*, 2011). Recent studies suggest that small scale processes such as precipitation (Pauluis and Dias, 2012) may significantly contribute to \bar{D} , which might therefore be considerably underestimated. Furthermore, the knowledge of how the Lorenz energy cycle will change in a warming scenario is an important metric to understand changes in future large scale circulation. Numerical simulations show that a CO₂ doubling causes a decrease of \bar{G} of nearly 10% (Lucarini *et al.*, 2010). Warming patterns can alter G either by affecting the gross static stability γ or the meridional temperature/diabatic heating distribution. Hernandez-Deckers and von Storch (2012) show that the decrease in G is mostly associated with changes in the gross static stability changes (i.e. in γ) rather than with meridional temperature gradient changes.

Another aspect to be considered is that usually the intensity of the Lorenz energy cycle is formulated assuming hydrostatic conditions and is computed for models that do not treat explicitly convection, but rather parametrize it with some sort of adjustment scheme. Therefore, the Lorenz energy cycle in itself neglects any systematic transfer of potential into kinetic energy occurring through non-hydrostatic, small scale motions. Obviously, the thermodynamics behind the set-up of organized convective motions can be framed in terms of an energy cycle similar to Lorenz', and requires a separated treatment. See the comments in Steinheimer *et al.* (2008).

The oceans' energy cycle is formally identical to that introduced for the atmosphere, with the only difference that generation of kinetic energy due to wind stresses at the surface and dissipation of potential energy due

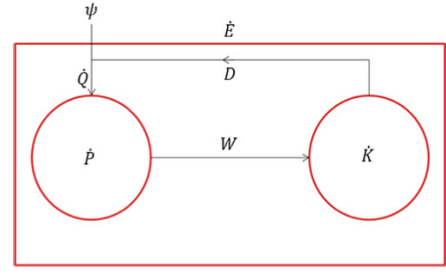


FIG. 10 Schematic figure showing atmospheric potential P and kinetic K reservoirs and the transfer processes (ψ, W, D) between them. $\dot{Q} = \psi + D$ is the total diabatic heating.

to molecular and small scale eddy mixing are not negligible (Peixoto and Oort, 1992) and therefore must be accounted for. As opposed to the atmospheric case, the oceanic energy cycle is powered mostly by an input of kinetic energy, and not of available potential energy. The oceanic Lorenz's energy cycle is still poorly understood from a theoretical point of view (Tailleux, 2013) and the various dissipation and generation terms are highly uncertain within the $(1 - 2) \times 10^{-2} \text{ W m}^{-2}$ range (Oort *et al.*, 1994; Storch *et al.*, 2012).

1. Heat engine and efficiency

By defining the total diabatic heating $\dot{q} = \dot{q}_{nf} + \rho\epsilon^2$ and splitting the atmospheric domain V into the subdomain V^+ in which $\dot{q} = \dot{q}^+ > 0$, and V^- , where $\dot{q} = \dot{q}^- < 0$, it can be seen from equation (73) that:

$$\bar{W} = \int_{V^+} \overline{\dot{q}^+ \rho} dV + \int_{V^-} \overline{\dot{q}^- \rho} dV \equiv \bar{\Phi}^+ + \bar{\Phi}^-, \quad (75)$$

with $\bar{\Phi}^+ > 0$ and $\bar{\Phi}^- < 0$ by definition. Therefore the atmosphere can be interpreted as a heat engine, in which $\bar{\Phi}^+$ and $\bar{\Phi}^-$ are the net heat gain and loss, and W the mechanical work. The efficiency of the atmospheric heat engine, i.e. the capability of generating mechanical work given a certain heat input, can therefore be defined as:

$$\eta = (\bar{\Phi}^+ + \bar{\Phi}^-) / (\bar{\Phi}^+) = \bar{W} / \bar{\Phi}^+. \quad (76)$$

The analogy between the atmosphere and a (Carnot) heat engine can be pushed further if we introduce the total rate of entropy change of the system, $\dot{S} = \int \dot{q}/T \rho dV = \dot{S}^+ + \dot{S}^-$. In a steady state the following expression holds:

$$\bar{S} = \frac{\bar{\Phi}^+}{T^+} + \frac{\bar{\Phi}^-}{T^-} = 0, \quad (77)$$

where $T^\pm \equiv \bar{\Phi}^\pm / \int_{V^\pm} \overline{\dot{q}^\pm / T \rho} dV$ from which it follows that $\eta = 1 - T^- / T^+$.

Johnson's approach generalizes to the global circulation similar heat engine theories previously used to characterize hurricane dynamics (Emanuel, 1991). In Emanuel's theory a mature hurricane is depicted as an ideal Carnot engine driven by the thermal disequilibrium between the sea-surface temperature T_s and the cooling temperature T_0 with an efficiency $1 - T_0/T_s \approx 1/3$. A similar approach was extended also to moist convection (Emanuel and Bister, 1996; Rennò and Ingersoll, 1996) for determining the the wind speed performed by the convective system for a certain rate of heat input F_{in} from the sea, $W = F_{in}(1 - T_0/T_s)$. Such an approach has been used to study large scale, open systems (e.g. Hadley cell, Adams and Rennò, 2005), and a grand goal seems the possibility of providing a thermodynamic theory of monsoonal circulation extending the results by Johnson (1989).

There are many, different definitions of efficiency used to characterize global circulations (Ambaum, 2010; Johnson, 2000; Perna et al., 2012; Schubert and Mitchell, 2013). As a future perspective, it would be desirable, from a theoretical point of view, to reconcile these definitions of thermodynamic efficiency and understand their differences.

2. Entropy production

More insight can be gained if we split \dot{S} into the sum of two contributions, $\dot{S} = \dot{S}_e + \dot{S}_i$, where \dot{S}_e is associated with the entropy fluxes with the surroundings and $\dot{S}_i \geq 0$ with internal irreversible processes (deGroot and Mazur, 1984). The term \dot{S}_e is associated with a certain amount of external heat \dot{q} added to the system by radiation (Goody, 2000), therefore the previous statement can be written, according to Clausius' formulation, as:

$$\dot{S} = \int \frac{\dot{q}}{T} \rho dV + \dot{S}_i, \quad \dot{S}_i \geq 0. \quad (78)$$

For a steady state $\overline{\dot{S}} = 0$, hence $\overline{\dot{S}_e} \leq 0$ (which is the analogue of Clausius' inequality $\oint \delta Q/T \leq 0$) implying that non-equilibrium systems must export entropy to the surroundings in order to maintain their patterns of flows and associated gradients.

In the case of the atmosphere, $\dot{S}_i = \dot{S}_{fric} + \dot{S}_{hyd} + \dot{S}_{diff}$, that is the sum of contributions associated with frictional heating, hydrological cycle (diffusion of water and phase-changes) and heat diffusion respectively. Entropy production due to heat diffusion is generally small (≈ 2 mW m⁻² K⁻¹, (Kleidon, 2009)) and associated mostly with dry-convection occurring nearby the surface. Frictional heating is associated with turbulent energy cascade bringing kinetic energy from large scales down to scales (millimeters or less for geophysical flows) where viscosity can act and $\overline{\dot{S}_{fric}} = \int \epsilon^2/T \rho dV \approx 10$ mW m⁻² K⁻¹

(Fraedrich and Lunkeit, 2008; Pascale et al., 2011). Pauluis and Dias (2012) argued that another large source of frictional dissipation (comparable to \dot{S}_{fric}) comes from shears surrounding falling hydrometeors. Finally, \dot{S}_{hyd} is due to irreversible processes associated with the hydrological cycle – evaporation of liquid water in unsaturated air, condensation of water vapour in supersaturated air and molecular diffusion of water vapour (Pauluis and Held, 2002a,b) and requires the knowledge of relative humidity \mathcal{H} and the molecular fluxes of water \mathbf{J}_v :

$$\begin{aligned} \dot{S}_{hyd} = & \int (C - E)R(\ln \mathcal{H} + \mathbf{J}_v \cdot \nabla p_w) dV \\ & - \int_{z=0} J_{v,z} R \ln \mathcal{H}. \end{aligned} \quad (79)$$

An indirect estimate of (79) can be obtained from the entropy budget for the water substance $\dot{S}^w = F_l/T + \dot{S}_{hyd}$ (Pauluis and Held, 2002b), where \dot{S}^w is the rate of change of entropy of water substance and F_l the amount of heat per time that the water substance receives from its environment (i.e. through evaporation and condensation ≈ 80 W m⁻²). For a steady state $\overline{\dot{S}^w} = 0$ and so $\overline{\dot{S}_{hyd}} = \overline{F_l(1/T_s - 1/T_a)} \approx 37$ mW m⁻² K⁻¹ (Pascale et al., 2011). Furthermore, in atmospheric models aphysical entropy sources due to diffusive/dispersive numerical advection schemes are also present (Johnson, 1997). Detailed estimates of the entropy budget of the climate system and of the material entropy production ($\overline{\dot{S}_i} \approx 50$ mW m⁻² K⁻¹) can be found in (Goody, 2000; Pascale et al., 2011). Oceanic entropy production due to small-scale mixing gives a small contribution (≈ 1 mW m⁻² K⁻¹) to $\overline{\dot{S}_i}$ (Pascale et al., 2011).

Furthermore, since $\overline{\dot{S}_i} = -\overline{\dot{S}_e}$, an indirect estimation of the material entropy production may be obtained as soon as the outgoing entropy fluxes are known. In the case of the climate systems, for example, this requires the knowledge of the radiative entropy fluxes. It is immediately understood the direct method may be, in principle, applied also to other planets (for which radiative fluxes is the only thing we can know) in order to infer information about their dissipative processes in their interior (Schubert and Mitchell, 2013). Starting from eq. (78) (Lucarini et al., 2011) derived an approximate relation for $\overline{\dot{S}_i}$ based only on 2-D radiative fluxes which permits to decompose $\overline{\dot{S}_i}$ into the sum of contributions due to horizontal and vertical processes (Pascale et al., 2012).

D. Applications and future perspectives

1. Bistability and tipping points

Based on the evidence supported by Hoffman and Schrag (2002) and from numerical models (Budyko, 1969;

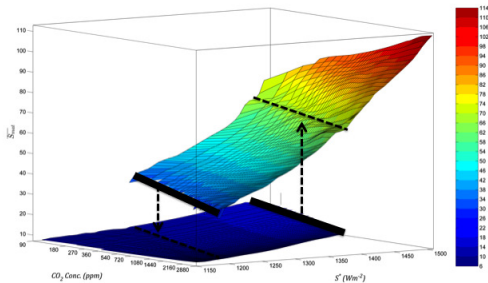


FIG. 11 Material entropy production ($\text{mW m}^{-2} \text{K}^{-1}$) as a function of solar constant S^* and the CO_2 concentration. The transition $\text{SB} \rightarrow \text{W}$ and $\text{W} \rightarrow \text{SB}$ are marked with dashed arrows starting from the tipping point regions (courtesy of R. Boschi, Universität Hamburg).

(Ghil, 1976; Sellers, 1969), it is expected that the Earth is potentially capable of supporting multiple steady states for the same values of some parameters such as, for example, the solar constant. Such states are the presently observed *warm* state (W), and the entirely ice covered *Snowball Earth* state (SB). This is due to the presence of two disjoint strange (chaotic) attractors. The $\text{W} \rightarrow \text{SB}$ and $\text{SB} \rightarrow \text{W}$ transitions are due, mathematically, to the catastrophic disappearance of one of the two strange attractors (Arnold, 1992) and, physically, to the positive ice-albedo feedback. The SB condition, which might be a common feature also of Earth-like planets, hardly allows for the presence of life, so this issue is of extreme relevance for defining habitability condition in extraterrestrial planets.

PLASIM (Fraedrich et al., 2005), a general circulation model of intermediate complexity, was used by Boschi et al. (2013); Lucarini et al. (2013) to reconstruct an extensive portion of the region of multistability in the plane described by the parameters $(S^*, [\text{CO}_2])$. The surface temperature $T_s(S^*, [\text{CO}_2])$ is shown in Fig. 11. The boundary of the domain in the parametric space where two states are admissible correspond to the tipping points of the system.

The thermodynamical and dynamical properties of the W and SB states are largely different. In the W states, surface temperature are 40 – 60 K higher than in the corresponding SB state and the hydrological cycle dominates the dynamics. This leads to a material entropy production (Fig. 12) larger by a factor of 4 – order of $(40 - 60) \times 10^{-3} \text{ W m}^{-2} \text{ K}^{-1}$ vs. $(10 - 15) \times 10^{-3} \text{ W m}^{-2} \text{ K}^{-1}$ – with respect to the corresponding SB states (Boschi et al., 2013). The SB state is eminently a dry climate, with entropy production mostly due to sensible heat fluxes and dissipation of kinetic energy.

The response to increasing temperatures of the two states is rather different: the W states feature a decrease of the efficiency of the climate machine, as enhanced latent heat transports kill energy availability by reducing temperature gradients, while in the SB states the efficiency is increased, because warmer states are associated to lower static stability, which favors large scale atmospheric motions (Fig. IV.D.1). The entropy production increases for both states, but for different reasons: the system become more irreversible and less efficient in the case of W states, while stronger atmospheric motions lead to stronger dissipation and stronger energy transports in the case of SB states. A general property which has been found is that, in both regimes, the efficiency η increases for steady states getting closer to tipping points and dramatically drops at the transition to the new state belonging to the other attractor (Fig. IV.D.1). In a rather general thermodynamical context, this can be framed as follows: the efficiency gives a measure of how far from equilibrium the system is. The negative feedbacks tend to counteract the differential heating due to the stellar insolation pattern, thus leading the system closer to equilibrium. At the bifurcation point, the negative feedbacks are overcome by the positive feedbacks, so that the system makes a global transition to a new state, where, in turn, the negative feedbacks are more efficient in stabilizing the system (Boschi et al., 2013).

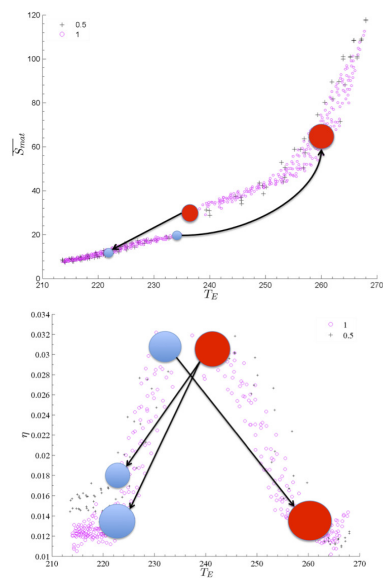


FIG. 12 Top: material entropy production ($10^{-3} \text{ W m}^{-2} \text{K}^{-1}$) vs. emission temperature T_E (K) for $\Omega = \Omega_{earth}$ (magenta) and $\Omega = 0.5\Omega_{earth}$ (black). Bottom: as in top figure but for efficiency (courtesy of R. Boschi).

Another interesting aspect is the determination of empirical functional relations between the main thermodynamical quantities and globally averaged emission temperature $T_E = (LW_{toa}/\sigma)^{1/4}$, as shown in Fig. 12. This

would permit to express nonequilibrium thermodynamical properties of the system in terms of parameters which are more directly accessible through measurements (*Lucarini et al.*, 2013).

2. Applications to planetary sciences

The discovery of hundreds of planets outside the solar system (exoplanets) (*Seager and Deming*, 2010) is extending the scope of planetary sciences towards the study of the so-called *exoclimates* (*Heng*, 2012a). A large number of the exoplanets discovered so far are tidally locked to their parental star, experiencing extreme stellar forcing on the dayside where temperature up to 2000 K can be reached. Starlight energy, deposited within the atmosphere at the planet’s dayside, is then transported by atmospheric circulation to the night side. Such a system, similarly to the Earth’s climate, works like a heat engine (Sect. IV.B.2, Sect. IV.C). The strength of the day-to-night enthalpy flux controls the ratio of outgoing longwave energy fluxes from the night and day side $\xi = LW_{night}/LW_{day}$, called efficiency of heat redistribution in the astrophysical literature. Observations through infrared light curves show that the hotter the planet, the more inefficient is the atmospheres at redistributing stellar energy leading to larger day-night temperature differences. Numerical simulations (*Perna et al.*, 2012) show that ξ varies between 0.2 (low heat redistribution) and 1 (full heat redistribution) and depends critically on the atmospheric optical properties and the intensity of the stellar irradiance. Relating this definition of efficiency with what proposed in Sect. IV.C would provide a link between energy conversion and energy transport in planetary atmospheres.

A thorough understanding of dissipative processes is fundamental for dealing with planetary atmospheres (*Goodman*, 2009; *Pascale et al.*, 2013). Dissipative processes are poorly known on Solar System planets (*Schubert and Mitchell*, 2013) and on exoplanets where processes unusual on Earth as Ohmic dissipation⁶ and cascading mechanisms such as shock wave breaking are believed to be common features (*Batygin and Stevenson*, 2010; *Heng*, 2012b).

⁶ In hot Jupiters temperatures may be very high (≥ 1500 K), allowing for thermal ionization (governed by the *Saha equation*) and thus fast-moving (in hot Jupiters winds $\sim 1 \text{ km s}^{-1}$) electric charges. This induces an electric current towards the interior of the planet, where energy is then converted into heat by ohmic dissipation.

V. CLIMATE RESPONSE AND PREDICTION

A. Introduction

In the previous section, we have investigated the climate as a non-equilibrium physical system and have emphasized the intimate relation between forcing, dissipation, energy conversion, and irreversibility. The same approach can be brought to a more theoretical level by taking the point of view of non-equilibrium statistical mechanics.

Non-equilibrium statistical mechanics provides the natural setting for investigating the mathematical properties of forced and dissipative chaotic systems, which live in a non-equilibrium steady state (NESS). In this state, typically, the phase space contracts, entropy is generated, and the predictability horizon is finite. Deviations from this behavior are possible, but extremely unlikely. Conceptually, non-equilibrium steady states are generated when a system is put in contact with reservoirs at different temperatures or chemical potentials, and one disregards the transient behaviors responsible for the relaxation processes (*Gallavotti*, 2006).

The science behind non-equilibrium statistical mechanical systems is still in its infancy, so that, as opposed to the equilibrium case, we are not able to predict the properties of a system given the parameters describing its internal dynamics and the boundary conditions, except in special cases where the dynamics is trivial.

It is then important to choose a suitable mathematical setting for being able to state some useful general results and compare numerical experiments with theory. It is advantageous to assume that the forced and dissipative systems under our consideration possess a unique Sinai-Ruelle-Bowen (SRB) measure (*Eckmann and Ruelle*, 1985; *Ruelle*, 1989; *Young*, 2002), which guarantees that, regardless of the initial state of the system, the steady state statistical properties are well defined and stable with respect to adding some noise. The invariant measure is supported on the attractor on the system, which is smooth along the unstable directions, and singular along the stable directions of the flow. In the very intuitive language of Lorenz, the attractor locally looks like the product of a manifold and a Cantor set. Moreover, the SRB measure can be considered as the zero-noise limit of the invariant measure of the original system perturbed by (small) stochastic forcing, and is thereby referred to as *physical measure*. Note that almost every time numerical simulations are performed, these hypotheses are implicitly assumed, because in the absence of an SRB measure, for most cases of practical interests it would make little sense to compute any statistical property of the system. In the case of multistable systems, possessing a disjoint attractor, one can assume that the statistical properties are well defined for all initial conditions belonging to the basin of attraction of the

same of the distinct piece of the attractor.

(Ruelle, 1997, 1998a,b, 2009) recently proved that in the case of an Axiom A system, its SRB measure, despite its geometrical complexity, has also an extremely fascinating degree of regularity. In fact, there is a smooth dependence of the SRB measure to small perturbations of the flow, and it is possible to derive corresponding explicit formulas. Such response formulas boils down to a Kubo-like (Kubo, 1957; Kubo et al., 1988) perturbative expression where the terms describing the linear and nonlinear response of the system can be written as expectation values of observables on the unperturbed SRB measure. This approach is especially useful for studying the impact of changes in the internal parameters of a system or of small modulations to the external forcing, and various studies have highlighted the practical relevance of Ruelle theory for studying what we may call the sensitivity of the system to small perturbations. Among the many results, one can mention the actual implementation of the response theory as an algorithm for predicting the finite and infinite time ensemble-averaged impact of forcings (Abramov and Majda, 2008), the provision of a connection between response theory and ensemble adjoint schemes (Eyink et al., 2004), the investigation of the frequency-dependent linear response of the system (Reick, 2002). Finally, some efforts have been directed at extending the analysis of the frequency dependent response to the nonlinear case (Lucarini, 2008) and on testing the robustness of the theory with simple chaotic models (Lucarini, 2009), and then applying the Ruelle's formulas to simple cases of geophysical relevance (Lucarini and Sarno, 2011). Recently the response theory has been used to study the impact of stochastic perturbations of chaotic systems (Lucarini, 2012) and derive rigorously parametrizations for reducing the complexity of multi-scale systems (Wouters and Lucarini, 2012) (see next Section).

B. Response formulas

Let's consider an Axiom A dynamical system whose evolution equation can be written as $\dot{x} = F(x)$ and let's assume that it possesses an invariant SRB measure $\rho^{(0)}(dx)$. Ruelle (1997, 1998a,b, 2009) has shown that if the system is weakly perturbed so that its evolution equation can be written as:

$$\dot{x} = F(x) + \Psi(x)T(t) \quad (80)$$

where $\Psi(x)$ is a weak time-independent forcing and $T(t)$ is its time modulation, it is possible to write the modification to the expectation value of a general smooth observable A as a perturbative series:

$$\rho(A)_t = \sum_{n=0}^{\infty} \rho^{(n)}(A)_t, \quad (81)$$

where $\rho^{(0)}(A)_t = \rho^{(0)}(A)$ is the expectation value of A according to the unperturbed invariant measure ρ^0 , while $\rho^{(n)}(A)_t$ with $n \geq 1$ represents the contribution due to n^{th} order processes and can be expressed as a n -uple convolution product:

$$\rho^{(n)}(A)_t = \int_{-\infty}^{\infty} d\tau_1 \dots \int_{-\infty}^{\infty} d\tau_n G_A^{(n)}(\tau_1, \dots, \tau_n) \times T(t - \tau_1) \dots T(t - \tau_n). \quad (82)$$

The integration kernel $G_A^{(n)}(\tau_1, \dots, \tau_n)$ is the n^{th} order Green function, which can be written as:

$$G_A^{(n)}(\tau_1, \dots, \tau_n) = \int \rho^{(0)}(dx) \Theta(\tau_1) \dots \Theta(\tau_n - \tau_{n-1}) \times \Lambda \Pi(\tau_n - \tau_{n-1}) \dots \Lambda \Pi(\tau_1) A(x). \quad (83)$$

where $\Lambda(\bullet) = \Psi \cdot \nabla(\bullet)$ describes the impact of the perturbation field and $\Pi(\sigma)$ is the unperturbed time evolution operator such that $\Pi(\sigma)K(x) = K(x(\sigma))$. The Green function obeys two fundamental properties

- its variables are time-ordered: if $j > k$, $\tau_j > \tau_k \rightarrow G_A^{(n)}(\tau_1, \dots, \tau_n) = 0$;
- the function is causal: $\tau_1 < 0 \rightarrow G_A^{(n)}(\tau_1, \dots, \tau_n) = 0$.

It is important to note that many authors suggest that, at all practical purposes, the validity of the response theory extends well beyond the (rich but somewhat limited) mathematical world of Axiom A systems if one consider reasonable physical systems. See discussions in (Eyink et al., 2004; Lacorata and Vulpiani, 2007; Marconi et al., 2008). One way to rationalize this statement comes from the so-called *Chaotic Hypothesis*: Axiom A systems can be considered as good *effective* models of actual systems with many degrees of freedom (Gallavotti, 1996).

Limiting our attention to the linear case we have:

$$\rho^{(1)}(A)_t = \int_{-\infty}^{+\infty} d\tau_1 G_A^{(1)}(\tau_1) T(t - \tau_1) \quad (84)$$

where the first order Green function can be expressed as follows:

$$G_A^{(1)}(\tau_1) = \int \rho^0(dx) \Theta(\tau_1) \Psi(x) \cdot \nabla A(x(\tau_1)), \quad (85)$$

In systems possessing a smooth invariant measure, like when equilibrium conditions apply or stochastic forcing is imposed, we can write $\rho^0(dx) = \rho^0(x)dx$, where $\rho^0(x)$ is the so-called *density*. In this case, we can rewrite Eq. 85 as follows:

$$\rho^{(1)}(A)_t = \int_{-\infty}^{+\infty} d\tau_1 \Theta(\tau_1) \int dx \rho^0(x) \times B(x) A(x(\tau_1)) T(t - \tau_1), \quad (86)$$

where $B(x) = -\nabla \cdot (\rho^0(x)\Psi(x)) / \rho^0(x)$. In other terms, one can predict the response at any time horizon t from the knowledge of the lagged correlation between the chosen observable A and the observable B , which depends on the invariant measure ρ^0 and on the perturbation vector field Ψ . Equation (86) provides a very general form of the Fluctuation-Dissipation Theorem (FDT) (*Lacorata and Vulpiani, 2007; Ruelle, 1998a*), which extends the results by (*Kubo, 1957*) obtained considering the classical case of equilibrium system immersed in a heat bath. Recently, the FTD for system possessing a smooth invariant measure result has been extended to the nonlinear case (*Lucarini and Colangeli, 2012*).

The more common forms of the FDT can be obtained by taking one or more of the following assumptions :

- the perturbation flow is the form $\Psi(x) = \epsilon \hat{x}_i$;
- the observable is of the form $A(x) = x_j$.

where x_k is the k^{th} component of the x vector and \hat{x}_k is the corresponding unit vector. In this case, Eq. 86 takes the form:

$$\rho^{(1)}(x_j)_t = -\epsilon \int_{-\infty}^{+\infty} d\tau_1 \Theta(\tau_1) \int dx \rho^0(x) \times \partial_i \log[\rho^0(x)] x_j(\tau_1) T(t - \tau_1), \quad (87)$$

If one takes the additional simplifying assumption that unperturbed invariant measure has a Gaussian form, so that $\rho^0(x) = 1/Z \exp(-\beta \sum_{j=1}^N x_j^2/2)$, where $\beta > 0$ and Z is a normalizing factor, we obtain:

$$\begin{aligned} \rho^{(1)}(x_j)_t &= \epsilon \beta \int_{-\infty}^{+\infty} d\tau_1 \Theta(\tau_1) \int dx \rho^0(x) \\ &\quad \times x_i x_j(\tau_1) T(t - \tau_1) \\ &= \epsilon \beta \int_{-\infty}^{+\infty} d\tau_1 \Theta(\tau_1) C_{i,j}(\tau_1) T(t - \tau_1), \quad (88) \end{aligned}$$

where $C_{i,j}$ is the lagged correlation between x_i and x_j in the unperturbed state. See also discussion in (*Cooper and Haynes, 2011; Cooper et al., 2013*).

Unfortunately, the link between linear response of the system to external perturbations and its internal fluctuations seems more elusive when the unperturbed state, as in general in case of non-equilibrium deterministic systems discussed above, has a singular invariant measure. In e.g. (*Ruelle, 2009*) it is shown that since the invariant measure is singular, the response of the system contains two contributions, such that the first may be expressed in terms of a correlation function evaluated with respect to the unperturbed dynamics along the space tangent to the attractor (unstable manifold) and is formally identical to what given in Eq. 86. This part of the response decays rapidly due to mixing. On the other hand, the second term, which has no equilibrium counterpart, depends on the dynamics along the stable manifold, and,

hence, it may not be determined from the unperturbed dynamics and is also quite difficult to compute numerically. The response to forcings along the stable directions can also be shown to converge as perturbations in these directions get damped exponentially fast by definition. These properties suggest the basic fact, already suggested heuristically by (*Lorenz, 1979*), that in the case of non-equilibrium systems internal and forced fluctuations of the system are not equivalent, the former being restricted to the unstable manifold only.

Despite such a serious mathematical difficulty, the application of FDT, even in extremely simplified, quasi-Gaussian, approximation, has enjoyed a good success in climate science, even if it is clear that the ability of FDT in predicting the response to perturbation depends critically on the choice of the observable of interest, on the length of the integrations needed for constructing the approximation of the invariant measure, and, of course, on the validity of the linear approximation (*Cooper and Haynes, 2011; Cooper et al., 2013; Gritsun and Branstator, 2007; Langen and Alexeev, 2005*).

There are, in fact, various ways to circumvent the problem of the rigorous non-equivalence between forced and free fluctuations. First, one can consider the smoothing effect due to unavoidable physical or numerical noise. On a more basic level, one can observe that when considering smooth, coarse-grained observables, one expect to see little influence of the fine structure of the invariant measure of chaotic deterministic systems, as projections from high-dimensional spaces to lower dimensional ones are involved (*Marconi et al., 2008*). In the case of climate problems, one expects that, for a given length of the control run needed for accumulating the statistics, the FDT will perform better in predicting the response of the system to perturbations if we consider as observable A quantities like the globally averaged surface temperature or the globally averaged emitted longwave radiation at the top of the atmosphere, than in predicting the response of, e.g. the surface temperature in an individual grid point. Moreover, it is indeed not obvious a priori to determine the range of forcings one which the response of a given observable will be closely approximated by the linear component of the response. Further comments can be found at the end of Sec. VI

C. Computing the Response

1. Spectroscopic method

If we select $T(t) = \epsilon \cos(\omega_0 t) = \epsilon/2(\exp(-i\omega_0 t) + \exp(i\omega_0 t))$ as modulating factor of the perturbation field

$\Psi(x)$, from equation Eq. 84 we derive:

$$\begin{aligned}\tilde{\rho}^{(1)}(A)_t &= \epsilon/2 \int_{-\infty}^{+\infty} d\tau_1 G_A^{(1)}(\tau_1) \exp(-i\omega_0(t - \tau_1)) \\ &+ \epsilon/2 \int_{-\infty}^{+\infty} d\tau_1 G_A^{(1)}(\tau_1) \exp(i\omega_0(t - \tau_1)) \\ &= \epsilon/2 \exp(-i\omega_0 t) \chi_A^{(1)}(\omega) + c.c.\end{aligned}\quad (89)$$

where $\chi_A^{(1)}(\omega_0)$ is the Fourier Transform of $G_A^{(1)}(t)$, usually referred to as linear susceptibility, evaluated at frequency $\omega = \omega_0$, and *c.c.* indicates complex conjugate. Therefore, under the hypothesis of linearity, by performing an ensemble of experiments where the forcing is of the form $T(t) = \epsilon \cos(\omega_0 t)$, we can extract the linear susceptibility at frequency ω by selecting the ω_0 component of the Fourier transform of the signal $\tilde{\rho}^{(1)}(A)_t$ obtained by taking the ensemble average of the difference between the time series of A in the perturbed and unperturbed case. By changing systematically the frequency ω of the forcing, one can reconstruct the susceptibility $\chi_A^{(1)}(\omega)$ on a chosen interval of frequencies. It is useful to recapitulate some useful features of the susceptibility:

- In general the response of a system to a forcing can be extremely different at for time scales of forcings. Therefore, one should use with great caution the concept of scale analysis. Moreover, $\lim_{\omega \rightarrow 0} \chi_A^{(1)}(\omega)$ is the static response of the system and is a positive number, which gives what is usually called the sensitivity.
- Resonances in the susceptibility function correspond to spectral ranges where the system is extremely sensitive to forcings. In Fig. 13 we show the real and imaginary part of the susceptibility for z variable of the (Lorenz, 1963) model - see Eqs .(49)-(51) - for the *classical* values of the parameters ($m = 1$, $\sigma = 10$, $r = 28$, $\beta = 8/3$) and a given choice of the forcing ($\Psi(x) = [0; x; 0]^T$, $T(t) = 2\epsilon \cos(\omega t)$). We find that for $\omega \sim 8.3$, a very peaked spectral feature is apparent. Such a resonance is due to the Unstable Periodic Orbits (UPOs) (Cvitanović, 1988) of the system with the corresponding period (Eckhardt and Ott, 1994). UPOs populate densely the attractors of chaotic systems and constitute the so-called skeleton of the dynamics. One can, in principle, reconstruct the whole statistics focussing on such special orbits then on the usual trajectories of the flow. In the case geophysical flows, UPOs have been associated to modes of low-frequency variability (Gritsun, 2008). One can, more qualitatively, associate resonance to positive feedbacks acting on time scales corresponding to the resonant frequency.
- While $|\chi_A^{(1)}(\omega)|$ measures the amplitude of the response of the system to perturbation at frequency

ω , $\arctan(\Im\{\chi_A^{(1)}(\omega)\}/\Re\{\chi_A^{(1)}(\omega)\})$ gives the phase delay between the forcing and the response, because the $\Re\{\chi_A^{(1)}(\omega)\}$ ($\Im\{\chi_A^{(1)}(\omega)\}$) gives the component of the response that is in phase (out of phase) with the forcing. Depending on the forcing, on the system, and on the observable, this angle can vary significantly even in a relatively small range of frequencies, as a result of resonances. There is, in general, nothing nonlinear in the presence of delays between forcing and response.

- The two components $\Im\{\chi_A^{(1)}(\omega)\}$ and $\Re\{\chi_A^{(1)}(\omega)\}$ are connected by integral equations, the so-called Kramers-Kronig relations (Lucarini, 2008, 2009; Lucarini et al., 2005; Ruelle, 2009). Such relations have their foundation in the causality of the Green function and establish a fundamental connection between the response at different time scales:

$$\Re\{\chi_A^{(1)}(\omega)\} = \frac{2}{\pi} P \int d\omega' \frac{\omega' \Im\{\chi_A^{(1)}(\omega')\}}{\omega'^2 - \omega^2}; \quad (90)$$

$$\Im\{\chi_A^{(1)}(\omega)\} = -\frac{2\omega}{\pi} P \int d\omega' \frac{\omega' \Re\{\chi_A^{(1)}(\omega')\}}{\omega'^2 - \omega^2}. \quad (91)$$

where P indicates that the integral is taken in principal part. In particular one finds that:

$$\Re\{\chi_A^{(1)}(0)\} = \frac{2}{\pi} \int d\omega' \frac{\Im\{\chi_A^{(1)}(\omega')\}}{\omega'}, \quad (92)$$

which provides a fundamental link between the static response - the sensitivity - and the out-of-phase response at all frequencies. An enormous literature exists in optics, acoustics, condensed matter physics, particle physics, signal processing on the theory and on the many applications of Kramer-Kronig relations and on the related *sum rules*, which provide integral constraints related to the asymptotic behavior of the susceptibility (Lucarini et al., 2005). This approach boils down to a spectroscopic investigation of the system and is thoroughly discussed, also in its numerical aspects, in (Lucarini, 2009; Lucarini and Sarno, 2011).

In Fig. 14 we present the real and imaginary part of the susceptibility of the mean energy e of the celebrated Lorenz (1996) model:

$$\frac{dx_i}{dt} = x_{i-1}(x_{i+1} - x_{i-2}) - x_i + F \quad (93)$$

where $i = 1, 2, \dots, N$, and the index i is cyclic so that $x_{i+N} = x_{i-N} = x_i$, and $e = 1/N \sum_{j=1}^N x_j^2/2$. The quadratic term in the equations simulates advection, the linear one represents thermal or mechanical damping and the constant one is an external forcing. The evolution

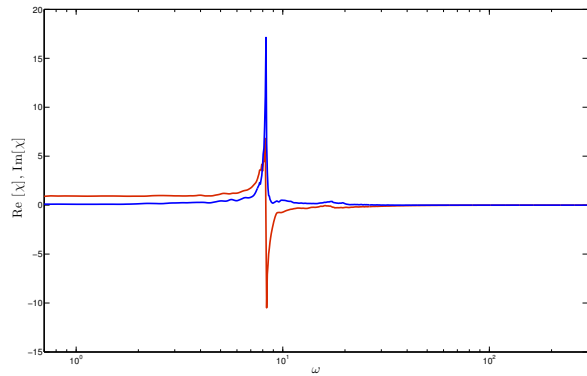


FIG. 13 Measured real (blue line) and imaginary (red line) part of the susceptibility z variable of the Lorenz 63 model. Data from *Lucarini* (2009)

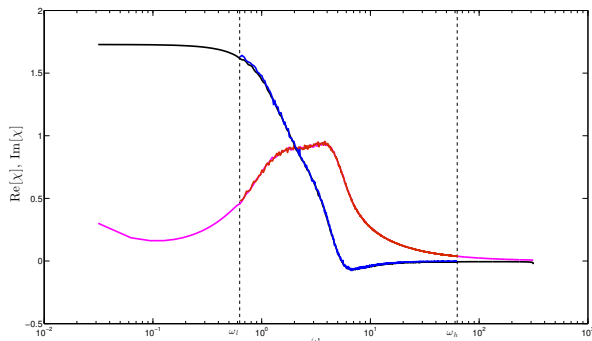


FIG. 14 Measured real (blue line) and imaginary (red line) part of the susceptibility for the average energy of the Lorenz 96 model. The rigorous extrapolation of the susceptibility obtained via Kramers-Kronig analysis is reported (real part: black line; imaginary part: magenta line). Data from *Lucarini and Sarno* (2011)

equations are invariant under $i \rightarrow i + 1$, so that the dynamics is the same for all variables. Please find details on the experiments in *Lucarini and Sarno* (2011), performed using $N = 40$ and $F = 8$. The system is perturbed by the vector field $\Psi(x) = [1; \dots; 1]^T$ modulated by $T(t) = 2\epsilon \cos(\omega t)$. The resulting real and imaginary part of $\chi_e^{(1)}(\omega)$ are reported in Fig. 14, together with the output of the data inversion performed via Kramers-Kronig relations. Once we obtain the susceptibility, as discussed in (*Lucarini and Sarno*, 2011), it is possible to derive the corresponding Green function by applying the inverse Fourier Transform. This is the first application of the Kramers-Kronig theory in a geophysical context.

2. Broadband forcing

If, instead, we select $T(t) = \delta(t)$, we derive from Eq. 85 that $\rho^{(1)}(A)_t = G_A^{(1)}(t)$, *i.e.* the Green function corresponds to the relaxation of an ensemble of trajectories of the system after a finite displacement along $\Psi(x)$. Obviously, we have that $\tilde{\rho}^{(1)}(A)_\omega = \chi_A^{(1)}(\omega)$, where the $\tilde{\rho}$ symbol, indicates, as customary, that a Fourier Transform has been applied, so that the Fourier Transform of the signal is the linear susceptibility. Therefore, using just one ensemble of experiments where the perturbation is described by an impulsive forcing, we can gather the same information on the response of the system which, in the previous case required an accurate sampling of different frequencies.

It is not always possible or advantageous to perform either of this class of experiments. Let's look at the problem from a slightly more general point of view., We apply the Fourier Transform to both sides of Eq. 84 and obtain:

$$\tilde{\rho}^{(1)}(A)_\omega = \chi_A^{(1)}(\omega) \tilde{T}(\omega) \quad (94)$$

Choosing a sine or cosine function with argument $\omega_0 t$ for the function $T(t)$ amounts to selecting as $\tilde{T}(\omega)$ the sum of two δ 's centered in $\omega = \omega_0$. Therefore, the input (forcing) allows only a small portion of the information to derived on the system from the output (response). Let's assume that we choose the modulation $T(t)$ such that $\tilde{T}(\omega)$ is not vanishing for any ω . A good option is to consider a broadband modulation, *i.e.* such that $\tilde{T}(\omega)$ is not vanishing for any ω and decreases slowly enough, *e.g.* like a power law. At this purpose, it is enough to choose a function which is differentiable only a finite numbers of times, including the case where there $T(t)$ is not continuous. If we perform an ensemble of simulations of the forced system, measure $\tilde{\rho}^{(1)}(A)_\omega$, we can readily derive:

$$\chi_A^{(1)}(\omega) = \frac{\tilde{\rho}^{(1)}(A)_\omega}{\tilde{T}(\omega)} \quad (95)$$

Therefore, one single set of experiments is, in fact all we need to do to learn about the linear response properties of the system for the observable A . If we want to predict the response at finite and infinite time of the system to forcing with the same spatial pattern $\Psi(x)$ but with different time modulation $R(t)$, we can derive $G_A^{(1)}(t)$ from $\chi_A^{(1)}(\omega)$ obtained via Eq. 95, and then plug it into Eq. 84. Alternatively, one can write:

$$\tilde{\rho}^{(1)}(A)_\omega^R = \tilde{\rho}^{(1)}(A)_\omega^T \frac{\tilde{R}(\omega)}{\tilde{T}(\omega)} \quad (96)$$

where the upper indices R and T have been inserted for clarity, and then compute the inverse Fourier transform to derive the response at all times.

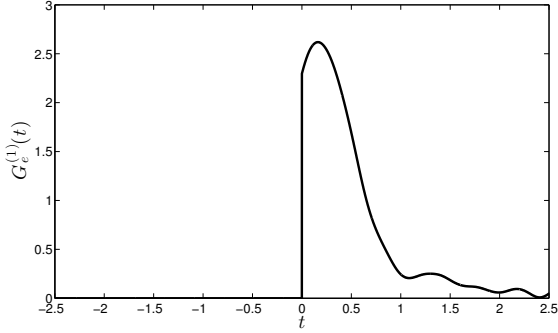


FIG. 15 Linear Green function $G_e^{(1)}(t)$ for the average energy e of the *Lorenz* (1996) model using the perturbation given in Eq. 97. Compare with Fig. 4 in *Lucarini and Sarno* (2011)

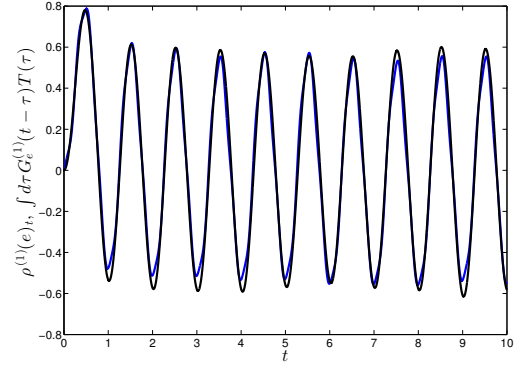


FIG. 16 Linear Green function $G_e^{(1)}(t)$ for the average energy e of the *Lorenz* (1996) model using the perturbation given in Eq. 97. Compare with Fig. 4 in *Lucarini and Sarno* (2011)

D. Prediction via Response theory

The real test of the quality of an experimentally derived linear Green function $G_A^{(1)}$ is the assessment of its ability to support predictions about the system's response to any temporal pattern of forcing $R(t)$. The real benefit of the broadband approach described here relies on exploiting linearity, and so deriving $G_A^{(1)}$ from just one ensemble of simulations, each performed with the same modulation $T(t)$. Computing the $G_A^{(1)}$ *per se* might be, in fact of little relevance ⁷.

At this regard, we have performed additional experiments on the (*Lorenz*, 1996) model mirroring what presented in Sec. V.C.1. In this case, we have chosen as time modulation $T(t) = \epsilon\Theta(t)$, whose spectrum is indeed broadband ($\tilde{T}(\omega)/\epsilon = \pi\delta(\omega) + iP[1/\omega]$). In this case, we have quite simply that:

$$G_e^{(1)}(t) = \frac{d}{dt}\rho^{(1)}(e)_t. \quad (97)$$

Using about 1/100 of the computing time needed in (*Lucarini and Sarno*, 2011), we have produced an estimate of the Green function of comparable quality; see Fig. 15. Additionally, we decided to check the predictive power of the reconstructed Green function given in Fig. 15 by testing its performance in predicting, through Eq. 84, the response of the system to a perturbation having temporal pattern given by $T(t) = \epsilon\sin(2\pi t)$ ($\epsilon = 0.25$). The results are presented in Fig. 16. The agreement between the measured value of $\rho^{(1)}(e)_t$ and the value predicted using $\int d\tau G_e^{(1)}(\tau)T(t-\tau)$ is remarkable. One must emphasize that the agreement is comparable if one selects $\epsilon = 1$, thus moving away from the linear regime.

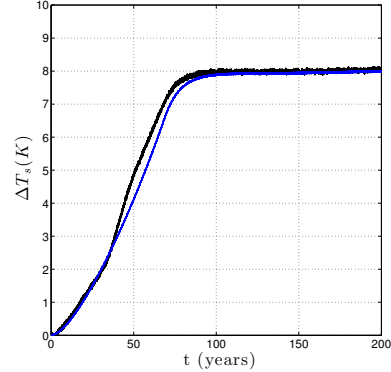


FIG. 17 Comparison between the observed response in the globally averaged surface temperature T_S to an exponential increase at 1% per year of CO_2 concentration from 360 to 720 ppm, with subsequent stabilization (black line), with the prediction performed using linear response theory (blue line). The experiment has been carried out using an ensemble of 200 climate simulations performed using the PLASIM model (*Fraedrich et al.*, 2005)

E. Climate Response, Climate Change prediction

Let's take inspiration from the previous example in order to get some results of stricter geophysical relevance: we want to perform predictions on the impact of increases in the CO_2 concentration on the globally averaged surface temperature as simulated by a climate model.

So, we consider that $\dot{x} = F(x)$ is the system of equations describing the discretized version of a given model of the continuum PDEs describing the evolution of the climate in a baseline scenario with set boundary conditions - and in particular the the value of the CO_2 concentration and of the solar constant. We assume, for simplicity, that system model does not feature daily or seasonal variations in the radiative input at the top of

⁷ The authors are thankful to F. Cooper for pointing out this issue.

the atmosphere. Let's choose for the observable A the globally averaged surface temperature of the planet T_S , let's consider as perturbation field $\Psi(x)$ the convergence of radiative fluxes due to change in the logarithm of the atmospheric CO_2 concentration. We want to be able to predict at finite and infinite time the response of the the system to one of the standard CO_2 forcing scenario given by the IPCC by performing an independent set of perturbed model integrations.

The test perturbation is modulated by the function $\epsilon\Theta(t)$, where ϵ is such that we double the amount of CO_2 concentration in the atmosphere. Our goal is to predict the climate response to the customary 1% increase of CO_2 concentration from the baseline value to its double. We select as baseline concentration $[CO_2] = 360 \text{ ppm}$. We perform 200 simulations, each lasting 200 years for both scenarios of CO_2 forcing. Our experiments are performed using PLASIM (*Fraedrich et al., 2005*) with a T21 spatial resolution, 10 vertical layers in the atmosphere, and swamp ocean having depth of 50 m.

From the time series of the ensemble mean of the change of $T_S - \rho^{(1)}(T_S)_t$ - resulting from the sudden increase in the CO_2 , we derive the Green function $G_{T_S}^{(1)}(t)$ using Eq. 97. Climate sensitivity is, in fact, defined by Eq. 92. Given the chosen pattern of forcing, we can rewrite is as follows:

$$\Delta_T = \Re\{\chi_A^{(1)}(0)\} = \frac{2}{\pi} \int d\omega' \Re\{\tilde{\rho}^{(1)}(T_S)_{\omega'}\}, \quad (98)$$

which relates climate response at all frequencies to its sensitivity.

We then convolute the Green function with the temporal pattern of forcing of the second set of experiments. Since our relevant control parameter is the logarithm of the CO_2 concentration, the pattern of forcing corresponding to an exponential increase is, in fact, a straight line. The results are presented in Fig. 17, where we compare the predicted pattern of increase (blue line) with the measure one (black line). The agreement is remarkable, both on the short and on the long time scales, while a discrepancy lower than 10% exists between 50 and 100 years lead time.

Apparently, despite all the nonlinear feedbacks of the climate model, the response to changes in the logarithm of CO_2 concentration can be accurately described by linear response theory at all time scales, not only in the static case, corresponding to climate sensitivity, which is our model, is extremely high as a result of lack of the seasonal cycle. Nonlinearity in the underlying equations and presence of strong positive and negative feedbacks do not rule out the possibility of constructing accurate methods for predicting the response. In fact, the methods described here could be extended to the nonlinear case by looking at the response in the frequency domain

(*Lucarini, 2008, 2009*), even if the data quality requirement is obviously stricter.

The result presented here suggests that, in fact, many of the scenarios of greenhouse gases concentration included in the IPCC reports (*IPCC, 2001, 2007, 2013*) may in fact be partly redundant, as for certain variables might be accurately described by linear response theory starting from just one scenario. Equations 95 - 96 constitute the basis for predicting climate response at all scales.

Obviously, with a given set of forced experiments, it is possible to derive the sensitivity to the the given forcing for as many climatic observables as desired. It is important to note that, for a given finite intensity ϵ of the forcing, the accuracy of the linear theory in describing the full response depends also on the observable of interest: the performance of the methods described here may be excellent for T_S but probably not for the precipitable water in the atmosphere, which, in first approximation, increases exponentially on the atmospheric temperature. Moreover, the signal to noise ratio and, consequently, the time scales over which predictive skill is good may change a lot from variable to variable.

F. Noise and Prediction

Of course, in order to talk about predictability, we need to specify what are the time scales over which we expect to have satisfactory predictive skills. In fact, linear response theory allows for deriving some scaling laws for addressing this matter. The main obstacle for achieving a good degree of predictability is the uncertainty on the estimate of response signal given in Eq. 94 from the outcomes of the numerical experiments because of the finiteness of the ensemble and of the duration of each numerical simulation.

The limits to predictability can be estimated as follows. As a result of the presence of a finite ensemble of N simulations of finite length L , the estimates of the absolute value of the response $|\tilde{\rho}^{(1)}(A)_{\omega}^{obs}|$ due to a forcing with spatial pattern $\Psi(x)$ and temporal pattern $T(t)$ differs from the true real and imaginary parts of the response $|\tilde{\rho}^{(1)}(A)_{\omega}|$ by a background function $\eta(\omega)$, which is a white noise of standard deviation $\sigma \sim \alpha N^{-1/2} L^{-1/2}$, where α is a constant, because the system decor relates exponentially fast thanks to its chaotic behavior. In the limit of either $N \rightarrow \infty$ or $L \rightarrow \infty$, if our estimate - as we expect - in unbiased, we obtain $|\tilde{\rho}^{(1)}(A)_{\omega}^{obs}| \rightarrow |\tilde{\rho}^{(1)}(A)_{\omega}|$.

From Eq. 95 we derive, that, if $|T(\omega)| \sim \beta\omega^{-\nu}$ for large values of ω , then the absolute value of $|\chi_A^{(1)}(\omega)^{obs}|$ is affected by a non stationary error due to undersampling, whose standard deviation increases as $\alpha\beta^{-1}N^{-1/2}L^{-1/2}\omega^{\nu}$. Let' assume that $|\chi_A^{(1)}(\omega)| \sim \kappa\omega^{-\gamma}$ as $\omega \rightarrow \infty$, with κ also a constant. Clearly, when ω is large enough, the absolute value of the true susceptibil-

ity $|\chi_A^{(1)}(\omega)|$ is smaller than the frequency dependent noise due to the unavoidable presence of $\eta(\omega)$. This happens when

$$\omega \gtrsim \omega_{crit} = \left(\frac{\alpha}{\beta\kappa}\right)^{-1/(\gamma+\nu)} N^{1/(2\gamma+2\nu)} L^{1/(2\gamma+2\nu)}. \quad (99)$$

In other terms, for frequencies larger than ω_{crit} , the estimate of $\hat{\chi}_A^{(1)}(\omega)$ is of little utility. This translates into the fact that the corresponding empirical $\hat{G}_e^{(1)}(t)$ will perform poorly in predicting changes occurring on time scales smaller than

$$t_{crit} \sim \left(\frac{\alpha}{\beta\kappa}\right)^{1/(\gamma+\nu)} N^{-1/(2\gamma+2\nu)} L^{-1/(2\gamma+2\nu)}. \quad (100)$$

Therefore, we are able to perform prediction on smaller and smaller scales if we have long integrations, many members of the ensemble, or a slow asymptotic decay of the susceptibility, and it is advantageous to choose, when probing the system, an observable which is as broadband as possible. Equations 99-100 provide a guidance on how the computational needs required to achieve predictive skills on a given time scale. Similar results can be obtained by looking at the impact of noise due to under-sampling on the real and imaginary part of the response and of the susceptibility.

VI. MULTISCALE SYSTEMS AND PARAMETRIZATIONS

A. Introduction

The climate is a complex system featuring non-trivial behavior on a large range of temporal and spatial scales (Lucarini, 2011; Peixoto and Oort, 1992; Vallis, 2006). It is clear that, no matter which are the available computing resources, we are able to simulate explicitly only the variable relevant for given ranges of spatial and temporal scales. Different choices of such ranges, in fact, correspond to different approximate theories of geophysical fluid dynamics aimed at describing specific phenomenologies, the most prominent case being, probably, the case of quasi-geostrophic theory.

A manifestation of the inability to treat ultraslow variability can be found in the usual practice in climate modeling of choosing fixed or externally driven boundary conditions, such as done when assuming a fixed extent for the land-based glaciers, and, consequently, for the sea-level, or imposing a specific path of CO_2 concentration for the atmosphere. See, at this regard, the distinction between *macroweather* and *climate* proposed by (Lovejoy and Schertzer, 2013). Instead, the impossibility of treating accurately fast processes requires the construction of so-called parametrizations able to account, at least approximately, the effect of the small scales on the large

scales, as a function of the properties of the large scale variables. The process of deriving parametrizations is also called model reduction or variable elimination.

Whereas deterministic and stochastic parametrizations are by now common in geophysical fluid dynamical models (Palmer and Williams, 2009), many of the approaches used up to now have been based on the existence of a time scale separation between microscopic and macroscopic processes. If one does assume a vast time-scale separation between the slow variables X and the fast variables Y , averaging and homogenization methods (Arnold, 2001; Kifer, 2004; Pavliotis and Stuart, 2008) allow for deriving an effective autonomous dynamics for the X variables, able to encompass the impact of the dynamics of the Y variables. In this prototypical case, one speaks of a two-level system where the X and Y variables constitute the two levels, respectively. A typical example of how this kind of theory can be used in climate science is the setting considered by Hasselmann, where fast *weather* systems influence slow *climate* dynamics. These methods will be reviewed in section VI.B.

Unfortunately, in many practical cases of interests geophysical fluid dynamics, such a scale separation does not exist, so that there is no spectral gap able to support univocally the identification of the X and Y variable. In fact, when the resolution of a numerical model is changed, all the parametrizations have to be re-tuned, because the set of resolved variables has changed. The possibility of constructing a robust theory of parametrizations would allow for constructing schemes applicable seamlessly to a model when its resolution is changed.

Here we will focus on analytical methods that allow one to derive reduced models from the dynamical equations of the full model. Projector operator techniques have been introduced in statistical mechanics with the goal of effectively removing the Y variables. In particular, considerable interest has been raised by the Mori-Zwanzig approach, through which a formal - albeit practically inaccessible - solution for the evolution of the X variables is derived (Zwanzig, 2001). These equations in general contain both a correlated noise term and a memory term. Some attempts have been made to make approximation to the Mori-Zwanzig projected equations to obtain practically useful equations. In applications of stochastic mode reduction in climate science, the memory term is usually not taken into account. This term could however be very relevant in systems without a time-scale separation, as for example in the parametrization of cloud formation in an atmospheric circulation model. The presence of memory in such systems has been discussed in (Bengtsson et al., 2013; Davies et al., 2009; Piriou et al., 2007). The Mori-Zwanzig projection operator technique and related approaches are described in section VI.D.

Besides a limit of infinite time scale separation, the limit of weak coupling between the different scales can also be considered. In this limit, the dynamics retains the

correlated noise and memory dependence that appeared in the Mori-Zwanzig reduced equations. The advantage of looking at this limit is however that the noise autocorrelation function and memory kernel can now be written as simple correlation and response functions of the unresolved dynamics. This approach will be reviewed in section VI.E

Many other parametrization methods have been proposed from a more heuristic point of view. Particularly relevant with respect to the current study are the results by (Kwasniok, 2012) indicating that non-Markovian parametrizations are superior to Markovian ones when a large time scale separation is absent. A similar conclusion can be reached from the work on empirical model reduction by Chekroun *et al.* (2011a), where non-Markovian models are fitted to data without a clear time scale separation.

B. Averaging and homogenization

When applying averaging and homogenization techniques, one considers dynamical systems where a small parameter ϵ controls the time scale separation between a slow and fast evolution in the system. The prototypical set of equations for such a problem is

$$\begin{aligned}\dot{x} &= f(x, y) \\ \dot{y} &= \frac{1}{\epsilon} g(x, y)\end{aligned}$$

The principle behind averaging can be considered similar to the law of large numbers. If the time scale separation becomes large, the fast system will go through its entire attractor on the time scale of evolution of the slow system. In the limit of ϵ going to zero, the slow system x will therefore 'see' all possible values of y . As in the law of large numbers, the overall effect of all these contributions can be substituted by one single value. It can be shown that for finite time T , the trajectory $x(t)$ converges to a solution of the equation

$$\dot{X} = F(X)$$

where $F(X) = \rho_{\infty, X}(f(X, y))$ is the averaged value of the tendency, the average taken over the invariant measure $\rho_{\infty, X}$ of the dynamical system

$$\dot{y} = g(X, y)$$

resulting for y when X is considered as a fixed forcing parameter. The convergence to the averaged solution depends on the type of the y dynamical system (stochastic or chaotic), on the coupling (full two-way or fast-to-slow only), and on the initial conditions (Kifer, 2009). Examples of dynamical systems can be constructed where for a large set of initial conditions of y , the solution for x does

not converge to the averaged solution (Kifer, 2008). Furthermore, if the y system has long time correlations, such as in a system with regime behaviour, the homogenized system may converge badly and an extension based on a truncation of the transfer operator has been proposed (Schütte *et al.*, 2004).

Let's consider a simple example system.

$$\begin{aligned}\dot{x} &= xy \\ \dot{y} &= -\frac{\lambda}{\epsilon} y + \frac{1}{\sqrt{\epsilon}} \frac{dW}{dt}\end{aligned}$$

The y system is an Ornstein-Uhlenbeck process, independent of x . The invariant measure of the fast y system is a Gaussian distribution with zero mean. Taking the average of $f(x, y) = xy$, we see that the averaged equation in this case is the uninteresting equation $\dot{X} = 0$.

This example immediately motivates the use of homogenization methods. Here one scales the equation to a longer time scale $\theta = \epsilon t$, the so called diffusive time scale and then performs the asymptotic expansion. Similarly to how correctly rescaling the sums of the law of large number leads to the more interesting central limit theorem instead, also in the setting of time scale separated systems, we get stochastic behavior on the diffusive time scale. For the example considered above, we get a weak convergence to a reduced stochastic differential equation for the X variable instead of the trivial dynamical system obtained before.

(Abramov, 2012) has recently presented an application of this method to deriving a simplified dynamics for a system of geophysical relevance. A study of averaging and homogenization for idealized climate models, with a range of examples, can be found in (Monahan and Culina, 2011). Another rather successful attempt in this direction is given in (Majda *et al.*, 2001).

A study of homogenization for geophysical flows was performed in Bouchet *et al.* (2013). The slow system is considered to be the evolution of zonal jets of a barotropic flow, which is forced by noise. The fast degrees of freedom are those representing the fast non-zonal turbulence. Homogenization has also been applied in (Dolaptchiev *et al.*, 2012) to the Burgers equation, where the slow variables are taken to be averages over large grid boxes and the fast variables are the subgrid variables.

When one wants to consider very large time scales (for examples times of the order of $\exp(1/\epsilon)$), one needs to look beyond the central limit type theorems of homogenization and consider so called large deviation results. These describe for example the transitions between disconnected attractors of the averaged equations (Kifer, 2009).

C. Dyson decomposition

The Dyson decomposition is an operator identity that allows to decompose the time evolution of observables of a dynamical system into a background evolution plus a term representing the effect of a perturbative vector field. This decomposition forms the basis of the Mori-Zwanzig method and the weak coupling method described in sections VI.E and VI.D.

Given a non-linear dynamical system $\dot{x} = F(x)$ on a manifold \mathcal{M} , the analysis of perturbations can be formally simplified by turning the problem into a linear equation for the evolution of observable functions $A : \mathcal{M} \rightarrow \mathbb{R}$. To this end, we define a linear differential operator $L(x) = (F(x) \cdot \nabla)$ called the Liouville operator, determining the time derivative of observables, dependent on time through a solution $x(t)$ of the dynamical system. We thus have that by the chain rule $\dot{A}(x(t)) = L(x(t))A(x(t))$. A solution of A over time is then given by $A(t) = \Pi(t)A(0)$ where $\Pi(t) = \exp(Lt)$. Although this equation does not tell us anything about the actual value of the solution, it does allow us to analyze perturbations, where the defining vector field F , and hence also L , are slightly altered.

As described *e.g.* in (Evans and Morriss, 2008), these perturbative relations can be easily derived formally in the resolvent formalism, by taking the Laplace transform of $\Pi(t)$:

$$\mathcal{L}\{\Pi\}(s) = \int_0^\infty dt \exp(Lt) \exp(-ts) = (s - L)^{-1} \quad (101)$$

If L consists of a perturbation around an operator L_0 , i.e. $L = L_0 + L_1$, with L_1 small in an appropriate sense, we can expand the Laplace transform using the equality

$$(A - B)^{-1} = A^{-1} + A^{-1}B(A - B)^{-1}. \quad (102)$$

In the case of the Laplace transform in Eq. 101, we take $A = s - L_0$ and $B = L_1$, so that the A^{-1} and $(A - B)^{-1}$ terms are themselves the Laplace transforms of $\Pi_0(t) = \exp(L_0 t)$ and $\Pi(t)$ respectively. Inverting the Laplace transform, the product of transforms gives a convolution term, resulting in the following decomposition of $\Pi(t)$:

$$\Pi(t) = \Pi_0(t) + \int_0^t d\tau \Pi_0(t - \tau) L_1 \Pi(\tau) \quad (103)$$

Another decomposition can be obtained when making use of the following equality for operator inverses:

$$(A - B)^{-1} = A^{-1} + (A - B)^{-1} B A^{-1}. \quad (104)$$

This gives rise to:

$$\Pi(t) = \Pi_0(t) + \int_0^t d\tau \Pi(t - \tau) L_1 \Pi_0(\tau) \quad (105)$$

These decompositions separate the evolution under the background evolution defined by L_0 from the effect of the perturbation L_1 .

As the right hand side of Eq. (103) and (105) still contain $\Pi(t)$, they can be iterated by to expand $\Pi(t) - \Pi_0(t)$ at different orders of the perturbation L_1 .

D. Projection operator technique

In the case of the Mori-Zwanzig approach (Mori *et al.*, 1974; Zwanzig, 1960, 1961) a projection is carried out on the level of the observables to remove unwanted, irrelevant and usually fast degrees of freedom. Here the expansion is performed around the evolution that involves only the relevant part of the phase space.

If a dynamical system is defined on a manifold \mathcal{M} , one defines a projection \mathcal{P} from the space of observable functions on the full phase space \mathcal{M} to a space of observables which are considered to contain only the interesting dynamics. Many different choices are possible; if the manifold \mathcal{M} consists for example of a product of submanifolds \mathcal{K} of relevant and \mathcal{L} of irrelevant variables, one can take a conditional expectation with respect to a measure on \mathcal{M} , given the value of the relevant variables $x \in \mathcal{K}$:

$$(\mathcal{P}A)(x) = \frac{\int_{\mathcal{N}} A(x, y) \rho(x, y) dy}{\int_{\mathcal{N}} \rho(x, y) dy}.$$

It is easily verified that this is a projection, i.e. $\mathcal{P}^2 = \mathcal{P}$ and that \mathcal{P} is orthogonal w.r.t the product defined by ρ : $\langle A, B \rangle = \int_{\mathcal{M}} \rho AB$. Another possible choice is a projection onto a set of functions on \mathcal{M} , such as linear functions of the coordinates in a Euclidean phase space.

The evolution operator L is now split into its projection $\mathcal{P}L$ onto the relevant space of observables and the complement $\mathcal{Q}L := (1 - \mathcal{P})L$. As described by (Zwanzig, 2001), a generalized Langevin equation can then be derived based on Eq. 105. We write the Liouville equation for an observable A as

$$\begin{aligned} \frac{dA(t)}{dt} &= LA(t) = e^{tL} LA \\ &= e^{tL} \mathcal{P}LA + e^{tL} \mathcal{Q}LA \end{aligned}$$

The factor $\exp(tL)$ in the second term can be further expanded by making use of Eq. 105 with $L_0 = \mathcal{Q}L$. This gives the following equation

$$\begin{aligned} \frac{dA(t)}{dt} &= e^{tL} \mathcal{P}LA \\ &+ (e^{t\mathcal{Q}L} + \int_0^t ds e^{(t-s)L} \mathcal{P}L e^{s\mathcal{Q}L}) \mathcal{Q}LA \end{aligned}$$

It is then argued (Zwanzig, 2001) that this equation is a generalization of the Langevin equation, where the second term is a correlated noise term dependent on the initial conditions of the irrelevant degrees of freedom and

the third term represent the memory of the system due to the presence of irrelevant variables that have interacted with the relevant ones in the past. Note that we have done nothing more than manipulating the original evolution equation $\dot{A} = LA$. Correspondingly, the Mori-Zwanzig equation in itself does not simplify the problem. In order to derive a set of equations that are useful for numerical simulations, assumptions need to be made about the dynamical system.

Several approximations to the Mori-Zwanzig equations have been proposed in the literature. There are the short and long memory approximations made in the method of optimal prediction (*Bernstein, 2007; Chorin and Stinis, 2006; Chorin and Hald, 2013; Chorin et al., 1998, 2000, 2002, 2006; Defrasne, 2004; Hald and Kupferman, 2001; Park et al., 2007*).

In the limit of an infinite time-scale separation between the relevant and irrelevant variables, the stochastic component of the parametrization can be represented as a white noise term, while the non-Markovian term vanishes, as the irrelevant variables decorrelate quickly, this brings us back to the homogenization method of section VI.B. For a discussion of the applicability of Mori-Zwanzig in climate sciences, see the paper by *Gottwald (2010)*.

E. Weakly coupled systems

We now consider dynamical systems consisting of two systems with a weak coupling. In this case an expansion of the dynamics can be made in orders of the coupling, giving insight into what properties of the coupled systems determines the memory kernel and correlated noise that appeared in the Mori-Zwanzig approach (*Wouters and Lucarini, 2012, 2013*).

A possible application of this theory in climate science can be found in the interaction between cloud formation and large scale atmospheric flow, where there is no distinct time scale separation, but instead the coupling could be considered as weak.

In this setting the background vector field F consists of a Cartesian product $(F_X, F_Y)^\top$ of the vector fields F_X and F_Y defining the autonomous X and Y dynamics. The perturbing vector field δF is a coupling $(\Psi_X, \Psi_Y)^\top$ between the two systems. The full dynamical system is given by

$$\begin{aligned}\frac{dX}{dt} &= F_X(X) + \Psi_X(X, Y) \\ \frac{dY}{dt} &= F_Y(Y) + \Psi_Y(X, Y)\end{aligned}\quad (106)$$

For simplicity of presentation, for now we consider the case where $\Psi_X(X, Y) = \Psi_X(Y)$ and $\Psi_Y(X, Y) = \Psi_Y(X)$. We will come back to the general case later.

Writing (106) in terms of observables using the chain rule, we have

$$\begin{aligned}\frac{dA(X, Y)}{dt} &= (L_X(X, Y) + L_Y(X, Y))A(X, Y) \\ &= (F_X(X) + \Psi_X(X, Y)) \cdot \nabla_X A(X, Y) \\ &\quad + (F_Y(Y) + \Psi_Y(X, Y)) \cdot \nabla_Y A(X, Y)\end{aligned}$$

where ∇_X and ∇_Y denote the gradients with respect to the variables in X and in Y respectively, $L_X = (F_X + \Psi_X)\nabla_X$ and $L_Y = (F_Y + \Psi_Y)\nabla_Y$.

We now do a calculation in the style of the Mori-Zwanzig one in Section VI.D for the dynamical system given in Eq. 106 and for observables A_X that only depend on the relevant variables X . We start the dynamical system at a time $-t$ in the past. The initial condition X_0 of the resolved variables is assumed to be known exactly. The state of the Y variables is not known exactly. Assuming that the coupled system is its invariant distribution ρ allows us to use the knowledge of X to further specify the distribution of Y . The Y variable is distributed according to the conditional distribution of ρ given X_0 . Expectation values of observables of Y are given by

$$\frac{\int dY B(Y) \rho(X_0, Y)}{\int dY \rho(X_0, Y)}$$

Since the coupling in the dynamical system corresponding to ρ is small, the invariant measure ρ is a perturbation around the uncoupled product measure $\rho_{0,X} \otimes \rho_{0,Y}$, where $\rho_{0,X}$ and $\rho_{0,Y}$ correspond to the unperturbed vector fields F_X and F_Y . Hence to zeroth order the conditional distribution of Y is simply $\rho_{0,Y}$.

We now try to understand what the distribution of tendencies of X is, given these initial conditions. As in Section VI.D, we first perform a projection of the evolution equation of A_X , in order to separate the X and Y variables. As projection, we choose the conditional expectation given by $\rho_{0,Y}$, i.e. $\mathcal{P}A = \int dY A(X, Y) \rho_{0,Y}(Y)$. Applying this projection to the time derivative of A_X decomposes the coupling $\Psi_X(Y)$ into its average value and fluctuations around it. We then apply an expansion in terms of Ψ to the evolution of the fluctuations.

The time derivative of A_X at $t = 0$ is given by

$$\begin{aligned}\frac{d}{dt} A_X(X, Y, t)|_{t=0} &= (L_X A_X)(X, Y) \\ &= ((\mathcal{P}L_X + \mathcal{Q}L_X)A_X)(X, Y) \\ &= (F_X(X) + \rho_Y(\Psi_X)) \nabla_X A_X(X) \\ &\quad + (\Psi_X(Y) - \rho_Y(\Psi_X)) \nabla_X A_X(X)\end{aligned}\quad (107)$$

We now want to find a formal solution for $\Psi_X(Y) - \rho_Y(\Psi_X)$ that we can insert into the previous equation.

The evolution of Ψ_X is given by

$$\begin{aligned}\Psi_X(Y) &= e^{t(L_X + L_Y)} \Psi_X(X_0, Y_0, -t) \\ &= e^{t(L_X + L_Y)} \Psi_X(Y_0)\end{aligned}$$

Making use of the decomposition of the Liouvillian $L = L_X + L_Y$ into $L_0(X_0, Y_0) = F_X(X_0)\nabla_X + F_Y(Y_0)\nabla_Y$ and $L_1(X_0, Y_0) = \Psi_X(Y_0)\nabla_X + \Psi_Y(X_0)\nabla_Y$, we derive by repeated use of Eq. 103 that

$$\begin{aligned} \Psi_X(Y) &= e^{t(L_0+L_1)}\Psi_X(Y_0) = e^{tL_0}\Psi_X(Y_0) \\ &+ \int_0^t d\tau e^{(t-\tau)L_0}L_1e^{\tau L_0}\Psi_X(Y_0) + O(L_1^2) \end{aligned} \quad (108)$$

Inserting this equation in (107), we get

$$\begin{aligned} & \left(\frac{d}{dt}A_X\right)(X, X_0, Y_0, t)|_{t=0} \\ &= (F_X(X) + \rho_Y(\Psi_X) + \tilde{\sigma}(t, Y_0))\nabla_X A_X(X) \\ &+ \left(\int_0^t d\tau \tilde{h}(t, \tau, X_0, Y_0)\right)\nabla_X A_X(X) \end{aligned}$$

where

$$\begin{aligned} \tilde{\sigma}(t, Y_0) &= e^{tF_Y(Y_0)\nabla_Y}\Psi_X(Y_0) - \rho_Y(\Psi_X) \\ \tilde{h}(t, \tau, X_0, Y_0) &= \Pi_0(t-\tau)L_1(X_0, Y_0)\Pi_0(\tau)\Psi_X(Y_0) \end{aligned}$$

Due to the commutation of $F_X\nabla_X$ and $F_Y\nabla_Y$, we have that

$$\begin{aligned} \tilde{h} &= \left(e^{(t-\tau)F_X\nabla_X}\Psi_Y(X_0)\right) \\ &\times e^{(t-\tau)F_X\nabla_X}\nabla_Y e^{\tau F_Y\nabla_Y}\Psi_X(Y_0) \end{aligned}$$

Now we can make use of the fact that Y is distributed according to ρ_Y , the invariant measure under the flow generated by F_Y . The average of $\tilde{\sigma}$ is then zero and the auto-correlation is given by the auto-correlation of the coupling function in the uncoupled Y system:

$$\rho_Y(\tilde{\sigma}(t, Y_0)) = 0$$

$$\begin{aligned} & \rho_Y(\tilde{\sigma}(t, Y_0)\tilde{\sigma}(t+\tau, Y_0)) \\ &= \rho_Y(\Psi_X(Y_0)e^{\tau F_Y\nabla_Y}\Psi_X(Y_0)) \end{aligned}$$

and the averaged memory kernel is given by a response function of the uncoupled Y system:

$$h = \rho_Y(\tilde{h}) = \Psi_Y(f_X^{t-\tau}(X_0))\rho_Y(\nabla_Y e^{\tau F_Y\nabla_Y}\Psi_X(Y_0)) \quad (109)$$

Proposing now a surrogate equation

$$\begin{aligned} \frac{d\tilde{X}(t)}{dt} &= F_X(\tilde{X}(t)) + M + \sigma(t) \\ &+ \int_0^\infty d\tau h(\tau, \tilde{X}(t-\tau)) \end{aligned} \quad (110)$$

we have that the average tendency of \tilde{X} to third order and its autocorrelation to second order in the coupling function correspond to those of the fully coupled system.

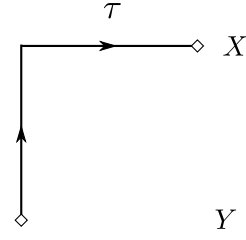


FIG. 18 Diagram describing the mean field effect of the Y variables on the X variables. Term M in Eq. 112.

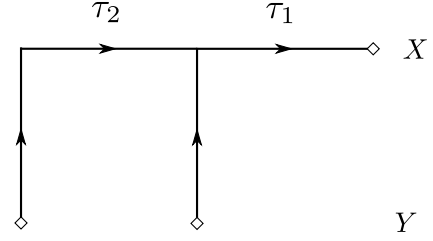


FIG. 19 Diagram describing the impact of fluctuations of the Y variables on the X variables. Term σ in Eq. 112.

F. Response Theory

The response theory is a rather flexible tool as the formalism can be applied in a variety of situations, as the perturbation flow $\Psi(x)$ can be of very different nature. Considering Eq. 106 a special case of such a forcing is the internal coupling of degrees of freedom given by $(\Psi_X, \Psi_Y)^\top$, to the unperturbed flow whose tendency is given by $(F_X, F_Y)^\top$. We can now use the formalism described in Section V for computing at all orders the change in the expectation value of $A = A(X)$ due to the coupling between the X and Y variables. After lengthy calculations, one obtain the explicit expression for

$$\rho(A)_t = \rho^0(A)_t + \rho^{(1)}(A)_t + \rho^{(2)}(A)_t + O(\Psi^3) \quad (111)$$

As shown in (*Wouters and Lucarini, 2012*), if one collects these first and second order responses to the coupling Ψ , an identical change in expectation values from the unperturbed ρ_0 up to third order in Ψ can be obtained by adding a Y -independent forcing to the tendency of the X variables as follows:

$$\begin{aligned} \frac{dX(t)}{dt} &= F_X(X(t)) + M + \sigma(t) \\ &+ \int_0^\infty d\tau h(\tau, X(t-\tau)) \end{aligned} \quad (112)$$

where $M = \rho_{0,Y}(\Psi_X)$ is an averaged version of the Y to X coupling, σ is a stochastic term, mimicking the two time correlation properties of the unresolved variables and h is a memory kernel that introduces the non-Markovianity. A diagrammatic representation of processes responsible that these three additional terms are parametrizing is given in Figs. 18-20. The memory effect

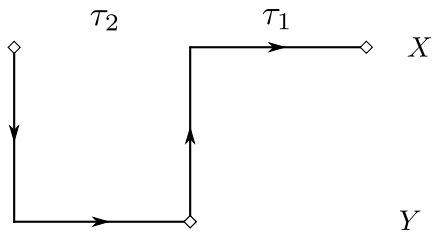


FIG. 20 Diagram describing the non-Markovian effect of the on the X variables on themselves, mediated by the Y variables. Term h in Eq. 112.

is present due to the finite time scale difference between resolved and unresolved variables.

It should be noted that the choice of parametrization is not unique. Any time-dependent forcing σ with the correct two-point time-correlations will give the right response up to second order. Also for the memory term there is some freedom. If the coupling functions Ψ_X and Ψ_Y are allowed to be dependent on both X and Y , the above analysis can still be carried out. For the case of separable couplings $\Psi_X(X, Y) = \Psi_{X,1}(X)\Psi_{X,2}(Y)$ and $\Psi_Y(X, Y) = \Psi_{Y,1}(X)\Psi_{Y,2}(Y)$ the average term becomes X dependent and the noise term becomes multiplicative instead of additive. An expression for more general couplings can be derived by decomposing the coupling functions into a basis of separable functions.

As obvious, Eqs. 110 and 112 are identical, which implies that, in terms of parametrization, it is equivalent to try to optimize the tendencies *in an averaged sense* or to try to minimize the bias in the statistical properties of any observable. Equations 110-112 provide a very general result concerning direct methods for constructing parametrizations from the statistical properties of unperturbed systems and the equivalence between the two results, obtained using rather distinct methods and concepts, suggest that there is a solid ground for exporting parametrizations developed for weather forecast into climate models.

The results contained in Eqs. 110 and 112 imply that, *up to second order*, the dynamics of the X variables contains a stochastic term, so that one can expect that the projection of the X variables of the invariant measure of the system given in Eq. 106 is, in fact to a good approximation, smooth, as a result of the regularizing effect due to noise. Therefore, the FDT applies when we consider observables $A = A(X)$, *i.e.* functions of the resolved, slow variables *only*. This provides a solid reason why the empirical application of the FDT in a context of climate dynamics has proved partially successful, and of why the degree of success depends critically on the climatic variable of interest.

VII. CONCLUSIONS

The main goal of this review paper is the provision of an overview of some ideas emerging at the interface between theoretical physics, mathematics, and climate science. The topics have been selected by the authors with the goal of covering (at least partially) relevant aspects of the deep symmetries of geophysical flows, of the processes by which they convert and transport energy and generate entropy, and of constructing relevant statistical mechanical models able to address fundamental issues like the response of the climate system to forcings, the representation of the interaction across scales, the definition of relevant physical quantities able to describe succinctly but accurately the dynamics of the system. The themes covered in the review also inform the development and testing of climate models of various degrees of complexity, by analyzing their physical and mathematical well-posedness and for constructing parametrizations of unresolved processes, and by putting the basis for constructing diagnostic tools able to capture the most relevant climate processes.

The Nambu formulation of geophysical fluid dynamics explored in Sec. II emphasizes the existence, in the inviscid case, of non-trivial conserved quantities that are embedded in the equations of motion. Such quantities - which include potential vorticity in the three dimensional case - play a fundamental role, analogous to energy's, in the description of the state of the system and can be regarded as observables of great relevance also in the case where dissipation and forcing are present. Moreover, the Nambu formalism suggests us ways for devising very accurate numerical schemes, which do not have spurious diffusive behavior.

The symmetry properties of the flow in the inviscid limit allow the construction of the ensembles describing the equilibrium statistical mechanical properties of the geophysical flows (Sec. III), where the vorticity - in the two dimensional case - plays the role of the most important physical quantity. Starting from the classical construction due to Onsager of the gas of interacting vortices, the theory leads us to construct a theory of barotropic and baroclinic QG turbulence.

Taking the point of view of non-equilibrium system, the description of the climate system is enriched as the presence of gradients of physical quantities like temperature and chemical concentrations - in first instance due to the inhomogeneity of the incoming solar radiation, of the optical properties of the geophysical fluids, and of the boundary conditions- supports the possibility of work being performed, resulting in organized fluid motions. In Sec. IV the analysis of the energy and entropy budgets of the climate system is shown to provide a comprehensive picture of climate dynamics, with promising outlook in terms of investigation of the climate tipping points and as a method for studying the properties of general planetary

atmospheres.

Section V introduces some basic concepts of non-equilibrium statistical mechanics, connecting the macroscopic properties described in the previous section to the features of the family of chaotic dynamical systems which constitute the backbone of the mathematical description of non-equilibrium systems. For such systems, the relationship between internal fluctuations and response to forcings is studied with the goal of developing methods for predicting climate change. After clarifying the conditions under which the fluctuation-dissipation theorem is valid, we show for the first time examples of successful climate prediction for decadal and longer time scales. In this sense, we show that the problem of climate change is mathematically well-posed.

Non-equilibrium statistical mechanics is also the subject of Sec. VI, where we show how the formalism of Mori-Zwanzig projection operator supports the provision of rigorous methods for constructing parametrizations of unresolved processes. It is possible to derive a surrogate dynamics for the coarse grained variable of interest for climatic purposes, incorporating, as result of the coupling with the small scale, fast variables, a deterministic, a stochastic, and a non-Markovian contribution, which add to the unperturbed dynamics. The same results can be obtained using the response theory described in Sec. V, thus showing that the construction of parametrizations for weather and for climate models should have common ground.

Among the many topics and aspects left out of this review, we need to mention recent developments aimed at connecting the complementary, rather than opposing (*Lorenz, 1963*) and (*Hasselmann, 1976*) perspectives on complex dynamics dynamics, which focus on deterministic chaos and stochastic perturbations to dynamical systems, respectively. We refer in particular to the idea of constructing time-dependent measures for non autonomous dynamical systems (*Chekroun et al., 2011b*) through the introduction of the so-called *pullback attractor*, which is the geometrical object the trajectories initialized in a distant past tend to at time t with probability 1 as a result of the contracting dynamics. Such an object is not invariant with time, as a result of the time-dependent forcing, but, under suitable conditions on the properties of the dynamical system, the supported measure has at each instant properties similar to those of the (invariant) SRB measure one can construct for, e.g. autonomous Axiom A dynamical (*Ruelle, 1989*). Such an approach allows for treating in a coherent way the presence of modulations in the dynamics of the system, without the need of applying response formulas or of assuming time-scale separations, and in particular allows for analyzing the case where the forcing is stochastic, leading to the concept of random attractor (*Arnold, 1988*). On a different line of research, it is instead possible to use Ruelle response theory for computing the impact of adding

stochastic noise on chaotic dynamical systems (*Lucarini, 2012*). One finds the rate of convergence of the stochastically perturbed measure to the unperturbed one, and discovers the general result that adding noise enhances the power spectrum of any given observables at all frequencies. The difference between the power spectrum of the perturbed and unperturbed system can be used, mirroring a fluctuation-dissipation result, for computing the response of the system to deterministic perturbations.

The methods, the ideas, the perspectives presented in this paper are partially overlapping, partially complementary, partly in contrast. In particular, it is not obvious, as of today, whether it is more efficient to approach the problem of constructing a theory of climate dynamics starting from the framework of hamiltonian mechanics and quasi-equilibrium statistical mechanics or taking the point of view of dissipative chaotic dynamical systems, and of non-equilibrium statistical mechanics, and even the authors of this review disagree. The former approach can rely on much more powerful mathematical tools, while the latter is more realistic and epistemologically more correct, because, obviously, the climate is, indeed, a non-equilibrium system. Nonetheless, the experience accumulated in many other scientific branches (chemistry, acoustics, material science, optics, etc.) has shown that by suitably applying perturbation theory to equilibrium systems one can provide an extremely accurate description of non-equilibrium properties. Such a lack of unified perspective, of well-established paradigms, should be seen as sign of the vitality of many research perspectives in climate dynamics.

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