Statistical mechanics of the one-layer shallow water model

Abstract: In this report, we present a study of the one-layer shallow water equations. We first recall the associated hydrodynamics, then we show how the statistical theory of these equations is constructed, and the few analytical results associated. We subsequently present the main work of this internship, a brand-new numerical Monte-Carlo code developed to sample numerically the microcanonical measure of these equations according to the theory with a Creutz algorithm. The internship was a little short to get subsequent results from this algorithm, but we present the few first results obtained at the end of the report.

Mots clefs: Statistical mechanics, Shallow water model, Monte-Carlo numerical simulation, Creutz algorithm

Stage encadré par:
Freddy Bouchet
freddy.bouchet@ens-lyon.fr / tél. (+33) 4 72 72 86 40
Laboratoire de Physique de l’ENS de Lyon
46, allée d’Italie
F69007 Lyon, FRANCE
http://www.ens-lyon.fr/PHYSIQUE

August 12, 2012
Acknowledgements

I would like to thank my advisor Dr. Freddy Bouchet for his support and great help. Your guidance and constructive criticism were really helpful in the difficult task of developing a numerical code from scratch, which I had never done before.
I also thank Max Potters, who worked on this subject and developed the equivalent 2-dimensional Euler code. He gave me a clear explanation of his previous work, which mostly inspired mine.
Finally, thanks to my co-workers Jason Laurie, Cesare Nardini and Shamik Gupta, it was a pleasure working with you.

Contents

Introduction 3

1 Statistical mechanics of the shallow water equations 3
   1.1 The hydrodynamical equations .............................................. 3
   1.2 Conserved quantities .......................................................... 4
   1.3 Microcanonical problem ...................................................... 5
      1.3.1 Invariant measure and Liouville’s theorem for a system with \( N \) degrees of freedom ............... 5
      1.3.2 Invariant measure and formal Liouville’s theorem for the dynamics of a field ..................... 5
      1.3.3 Microcanonical theory ................................................ 7

2 Sampling the microcanonical measure numerically 8
   2.1 Definition of the algorithm .................................................. 8
   2.2 Numerical system ............................................................... 8
      2.2.1 Definition of the system ................................................ 8
      2.2.2 Dimensional analysis .................................................... 9
      2.2.3 Grid definitions ........................................................... 9
   2.3 Definition of the moves ...................................................... 11
      2.3.1 \( q \) move ................................................................. 11
      2.3.2 \( h \) move ................................................................. 11
      2.3.3 \( \eta \) move ............................................................... 12
      2.3.4 Area move ............................................................... 12
   2.4 Temperature computation using the Creutz algorithm .................. 13

3 First results 13
   3.1 Energy distribution ........................................................... 14
      3.1.1 First run: \( \epsilon_e = \epsilon_v = 0.1, F = 0.1 \) .............................. 14
      3.1.2 Second run: \( \epsilon_e = 0.1, \epsilon_v = 1.0, F = 0.1 \) ....................... 15
      3.1.3 Third run: \( \epsilon_e = \epsilon_v = 0.1, F = 0.5 \) .............................. 15
   3.2 \( h \) field analysis ............................................................. 16
      3.2.1 First run: \( \epsilon_e = \epsilon_v = 0.1, F = 0.1 \) .............................. 16
      3.2.2 Second run: \( \epsilon_e = 0.1, \epsilon_v = 1.0, F = 0.1 \) ....................... 16
      3.2.3 Third run: \( \epsilon_e = \epsilon_v = 0.1, F = 0.5 \) .............................. 17
   3.3 Absence of large-scale structures ......................................... 18
      3.3.1 First run: \( \epsilon_e = \epsilon_v = 0.1, F = 0.1 \) .............................. 18
      3.3.2 Second run: \( \epsilon_e = 0.1, \epsilon_v = 1.0, F = 0.1 \) ....................... 18
      3.3.3 Third run: \( \epsilon_e = \epsilon_v = 0.1, F = 0.5 \) .............................. 19

Conclusion 20

A Canonical theory 21
   A.1 Constraints ................................................................. 21
   A.2 Solution of the variational problem .................................... 21
Introduction

Geophysical flows are highly turbulent, yet they embody large-scale coherent structures such as ocean rings, jets, and large-scale circulations. Understanding how these structures appear and predicting their shapes are major theoretical challenges.

The equilibrium statistical mechanics approach to geophysical flows is a powerful complement to more conventional theoretical and numerical methods [3]. The main idea is to consider a Hamiltonian set of hydrodynamical equations (e.g. Euler) as equations for microstates and construct the statistical mechanics for such a system; one can then determine the statistics of the accessible microstates under constraints given by conserved quantities, such as the energy, and therefore determine the local statistical properties of the system.

In 3-dimensional turbulent flows, large-scale structures cannot exist over a long period of time due to the Kolmogorov cascade, which transports the energy from large to small scales. In 2-dimensional flows, new motion invariants appear: the Casimir invariants. They constrain the accessible phase space to a set of microstates in which energy is mainly in the large scales. In the inertial limit, this method allows one to describe, with only a few thermodynamical parameters, the long-time behavior of the largest scales of the flow.

Recent studies of 2D Euler and quasi-geostrophic equations with this statistical approach provide encouraging results: a model of the Great Red Spot of Jupiter [1], an explanation of the drift properties of ocean rings [2], the inertial structure of mid-basin eastward jets [2], and so on.

In this internship, we try to extend this approach to a more complex hydrodynamic set of equations: the one-layer shallow-water model. This model is particularly useful for meteorological purposes, the multi-layer shallow-water model being used to describe many geophysical phenomena. We describe the microcanonical ensemble of this system in section 1, then we explain the numerical scheme used for sampling the microcanonical measure in section 2: this was the main body of work accomplished during this internship. We present the first results in section 3.

1 Statistical mechanics of the shallow water equations

1.1 The hydrodynamical equations

The one-layer Shallow water equations represent the motion of a thin layer of an incompressible fluid with uniform density $\rho$. The assumption of the model is that the motion is nearly two-dimensional: the typical horizontal scales are supposed to be much larger than the vertical width of the layer. As a consequence, the vertical component of the speed is small compared to the horizontal components. In the shallow-water model, the speed is considered to be purely horizontal at leading order, as shown in Fig.1:

![Shallow water model diagram](image)

A heuristic method for deriving the hydrodynamical equations is to write down the conservation of mass and momentum in 3 dimensions, and then to neglect the vertical component of the speed. Assuming that the Coriolis Force must be taken into account (application to geophysical flows), that the vertical equation reduces to the hydrostatic balance, that there is no viscosity and that there is a flat bottom topography, these equations read:

$$\partial_t v + (v \cdot \nabla)v + f e_z \times v = -g \nabla h(x,y)$$ (1.1)
$$\partial_t h + \nabla \cdot (hv) = 0$$ (1.2)

where $f$ is the Coriolis parameter and $g$ is the gravitation acceleration. The Eq.(1.2) is the mass conservation for an incompressible two-dimensional flow. The right-hand side of Eq.(1.1) is the pressure term.

A more detailed derivation of these equations can also be obtained from the 3-dimensional Euler equation, assuming hydrostatic balance at leading order and that the typical horizontal scales are much larger than the vertical width [7]. Such an assumption is generally correct in geophysical flows where the Coriolis force strongly constraints the fluid in the vertical direction, as explained by the Proudman-Taylor theorem.
Equation Eq.(1.1) can be equivalently written in terms of other variables corresponding to the impulsion \( M = h \nu \):

\[
\begin{align*}
\partial_t M_x + \partial_x \left( \frac{M_x^2}{h} \right) + \partial_y \left( \frac{M_x M_y}{h} \right) + \partial_z \left( \frac{1}{2} gh^2 \right) - f M_y &= 0 \\
\partial_t M_y + \partial_y \left( \frac{M_y^2}{h} \right) + \partial_x \left( \frac{M_x M_y}{h} \right) + \partial_y \left( \frac{1}{2} gh^2 \right) + f M_x &= 0.
\end{align*}
\] (1.3)\hspace{1cm} (1.4)

We clearly see that, if there is no Coriolis term, Eq.(1.3) and (1.4) are conservation laws. This form is useful to construct the microcanonical measure of the system, as will be discussed further in Sec.1.3.

An interesting consequence of Eq.(1.1) and Eq.(1.2) is the conservation of the potential vorticity \( q = \frac{\omega + f}{h} \):

\[ \partial_t q + \nu \cdot \nabla q = 0 \] (1.5)

where \( \omega = (\nabla \times \nu) \cdot e_z \) is the vorticity. This can be obtained by deriving the expression for \( q \) with respect to the time and inserting the shallow-water equations [7].

## 1.2 Conserved quantities

The shallow water equations conserve some particular quantities; first of them, the energy per unit mass reads:

\[ E[\nu, h] = \frac{1}{2} \int_\mathcal{D} d^2 r \ h (\nu^2 + gh) \] (1.6)

where the first part is the kinetic energy and the second part is the gravitational potential energy. The kinetic part can be separated into a vortical and a divergent contribution: using the Helmholtz decomposition of the field \( h \nu \), one obtains by integration by parts:

\[ E_{\text{kin}}[\nu, h] = -\frac{1}{2} \int_\mathcal{D} d^2 r \ \left( \Psi(r) \omega(r) + \Phi(r) \delta(r) \right) \] (1.7)

where \( \omega = (\nabla \times \nu) \cdot e_z \) is the vorticity, \( \delta = \nabla \cdot \nu \) the divergence, and

\[ \begin{align*}
\Delta \Psi &= (\nabla \times (h \nu)) \cdot e_z \\
\Delta \Phi &= \nabla \cdot (h \nu) \\
h \nu &= -\nabla \Psi \times e_z + \nabla \phi.
\end{align*} \] (1.8)\hspace{1cm} (1.9)\hspace{1cm} (1.10)

The equations also conserve an infinite number of functionals, called the Casimir invariants, which read:

\[ C_s[q] = \int_\mathcal{D} d^2 r \ h \ s(q), \] (1.11)

where \( s \) is any sufficiently smooth function (Eq.(1.11) can be derived from Eq.(1.2) and (1.5)). The equivalent quantities for the Euler 2D model are responsible for the creation of large-scale structures, as they prevent the energy from cascading to smaller scales; they are directly linked to the conservation of the vorticity in Euler 2D, which is analogous to Eq.(1.5). In the shallow water model we expect these quantities to prevent the vortical energy (as defined by Eq.(1.7)) from cascading to smaller scales, but there is no a priori constraint on the divergent part of the field. Understanding how these Casimir invariants play a role on the flow is one of the aims of this statistical mechanics approach.

The Casimirs can be written in a more useful form. A special Casimir is:

\[ C(\sigma) = \int_\mathcal{D} d^2 r \ h \ H(-q + \sigma) \] (1.12)

where \( H \) is the Heaviside step function. \( C(\sigma) \) returns the volume (area weighted by \( h \)) occupied by all potential vorticity levels smaller or equal to \( \sigma \). \( C(\sigma) \) is an invariant for any \( \sigma \) and therefore any derivative of it as well. The distribution of potential vorticity is defined as \( D(\sigma) = C'(\sigma) \), where the prime denotes a derivation with respect to \( \sigma \). Therefore, \( D(\sigma) \) is also conserved by the dynamics. The expression \( D(\sigma) d\sigma \) designates the volume occupied by the potential vorticity levels in the range \( \sigma \leq q \leq \sigma + d\sigma \). Then, the Casimirs can be written in the form

\[ C_f[q] = \int d\sigma \ f(\sigma) D(\sigma). \] (1.13)

The conservation of all Casimirs, Eq.(1.11), is therefore equivalent to the conservation of \( D(\sigma) \).
1.3 Microcanonical problem

Let us now construct the microcanonical theory of the shallow water equations. An equilibrium statistical theory must be justified by the existence of an invariant measure over the phase space. If no invariant measure can be found, the statistical properties of the system are evolving over time, and then no statistical equilibrium can be defined. We first recall what an invariant measure is and how it is connected with the Liouville theorem. We then formally explain how it applies to a field, and we find the relevant microscopic variables of our problem. We finally compute the partition function for the shallow water equations in the microcanonical ensemble.

1.3.1 Invariant measure and Liouville’s theorem for a system with \( N \) degrees of freedom

Let us first consider a dynamical system in a space with a finite number \( N \) of degrees of freedom \( \{ \omega_i \}_{1 \leq i \leq N} \). We suppose that its dynamics is described by \( \dot{\omega}_i = F_i(\omega) \).

We consider a measure over the phase space, \( \mu \), with density \( f \). The average of an observable \( A \) over this measure is then defined as:

\[
\langle A \rangle = \mu(A) = \int \prod_{i=1}^{N} d\omega_i f(\omega) A(\omega_j),
\]

(1.14)

The measure \( \mu \) is called invariant for the dynamics if

\[
\frac{d}{dt} \mu(A) = 0 \quad \forall A
\]

(1.15)

which, after an integration by parts, is equivalent to:

\[
\int \prod_{i=1}^{N} d\omega_i \sum_{j=1}^{N} \frac{\partial}{\partial \omega_j} (f(\omega)F_j(\omega))A(\omega) = 0 \quad \forall A.
\]

(1.16)

Let us consider a vector field \( V(.) \) over the phase space. The divergence of \( V \) with respect to \( \mu \) is then defined as

\[
\nabla_f V = \frac{1}{f(\omega)} \sum_{j=1}^{N} \frac{\partial}{\partial \omega_j} (f(\omega)V_j(\omega)).
\]

(1.17)

Then a simple condition for \( \mu \) to be an invariant measure is

\[
\nabla_f F = 0.
\]

(1.18)

**Simple case of Hamiltonian dynamics**  In the simple case of Hamiltonian dynamics, the phase space is \( \{ x_i, p_i \} \), and the dynamics is described by

\[
\dot{x}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial x_i}.
\]

(1.19)

It is then very easy to verify that the uniform measure over the phase space, \( d\mu = \prod_{i=1}^{N} dx_i dp_i \) (corresponding to \( f = 1 \)) is invariant. This result is called the Liouville theorem.

1.3.2 Invariant measure and formal Liouville’s theorem for the dynamics of a field

**Formal Liouville theorem**  We consider the Hamiltonian dynamics for a field \( \omega \):

\[
\dot{\omega}(r) = F(\omega)[\omega].
\]

We consider a measure \( \mu \) over the space of fields. We assume \( \mu \) has a density \( f \) with respect to \( D[\omega] \), that would be a generalization of the Liouville measure. Such an object should be defined through discretization and a limit procedure. We do not consider this problem here. We look at a Liouville theorem derived through algebraic formal computations. We will call such a result a formal Liouville theorem.

The average of an observable \( A \) over this measure is then formally written as:

\[
\mu(A) = \int \frac{D[\omega]f[\omega]}{D\mu} A[\omega].
\]

(1.20)
Then, formally,
\[
\frac{d}{dt} \mu(A) = \int \mathcal{D}[\omega] f[\omega] \frac{d}{dt} ([A[\omega]]) = \int \mathcal{D}[\omega] f[\omega] \int \mathcal{D} \mathbf{r} \frac{\partial F(\mathbf{r})[\omega]}{\partial \omega(\mathbf{r})} \frac{\delta A}{\delta \omega(\mathbf{r})} = - \int \mathcal{D}[\omega] A[\omega] \int \mathcal{D} \mathbf{r} \frac{\delta}{\delta \omega(\mathbf{r})} \{ F[\omega] f[\omega] \}.
\]

Let us consider vector field \( V(.) \) over the phase space of fields \( \omega \). The divergence of \( V \) with respect to \( \mu \) is then defined as
\[
\nabla_f V = \frac{1}{f[\omega]} \int \mathcal{D} \mathbf{r} \frac{\delta}{\delta \omega(\mathbf{r})} \{ F(\mathbf{r})[\omega] f[\omega] \}.
\]

Then a simple condition for \( \mu \) to be an invariant measure is
\[
\nabla_f F = 0.
\]

Let us assume that if \( F \) can be written as the divergence of a vector over the physical space
\[
F(\mathbf{r})[\omega] = \nabla_r \cdot (G(\mathbf{r})[\omega])
\]
then
\[
\int \mathcal{D} \mathbf{r} \frac{\delta}{\delta \omega(\mathbf{r})} \{ F(\mathbf{r}) \} = - \int \mathcal{D} \mathbf{r} \nabla_r \cdot \left( \frac{\delta G}{\delta \omega(\mathbf{r})} \right).
\]

We can use Green formula and conclude that whenever boundary terms vanish, this expression will be zero. This will be the case for instance if we consider periodic boundary conditions, or if \( \frac{\delta G}{\delta \omega(\mathbf{r})} \cdot \mathbf{n} = 0 \) where \( \mathbf{n} \) is the unit vector normal to the boundary of the physical domain \( \mathcal{D} \). This last condition is fulfilled if \( G(\mathbf{r})[\omega] \cdot \mathbf{n} = 0 \). In those cases, we conclude that the Liouville theorem holds for the formal measure \( d\mu = \mathcal{D}[\omega] \).

**The 2D Euler case** In the case of incompressible Euler 2D, the evolution equation reads:
\[
\partial_t \omega = - \nabla \cdot (\omega \mathbf{v}).
\]

Then \( \mathbf{G} = -\omega \mathbf{v} \) and a formal Liouville theorem holds for the formal measure \( \mu \) with \( d\mu = \mathcal{D}[\omega] \).

**The case of the shallow water model** In the case of the shallow water model, the microscopic variables must be carefully chosen. It is quite easy to demonstrate the Liouville theorem for the variables \((M_x = h\nu_x, M_y = h\nu_y, h)\). Using those variables, the shallow water equations read:
\[
\begin{align*}
\partial_t M_x + \partial_x \left( \frac{M_x^2}{h} \right) + \partial_y \left( \frac{M_x M_y}{h} \right) + \partial_x \left( \frac{1}{2}gh^2 \right) - f M_y &= 0 \\
\partial_t M_y + \partial_y \left( \frac{M_y^2}{h} \right) + \partial_x \left( \frac{M_x M_y}{h} \right) + \partial_y \left( \frac{1}{2}gh^2 \right) + f M_x &= 0 \\
\partial_t h + \nabla \cdot (h \mathbf{v}) &= 0.
\end{align*}
\]

The fact that the part of the vector field describing the evolution of \( h \) is a divergence is straightforward. The contribution from \( M_x \) to the vector field divergence is:
\[
\int \mathcal{D} \mathbf{r} \frac{\delta}{\delta M_x(\mathbf{r})} \left[ - \nabla \cdot \left( \frac{M_x \mathbf{M}}{h} \right) + \partial_x \left( \frac{1}{2}gh^2 \right) + f M_y \right].
\]

The second and third terms in Eq.(1.27) vanish as they are independent of \( M_x \). The first term in Eq.(1.27) is the divergence of \( M_x \frac{\mathbf{M}}{h} \), it can thus be integrated using Green theorem. It gives a vanishing boundary contribution as the inpenetrability condition imposes \( \mathbf{M} \cdot \mathbf{n} = 0 \) on the domain boundary. For similar reasons, the contribution from \( M_y \) to the vector field divergence also vanishes.

We thus conclude that a formal Liouville theorem holds for the shallow water equations for the measure \( \mu \) with \( d\mu = \mathcal{D}[h] \mathcal{D}[M_x] \mathcal{D}[M_y] \).

A different invariant measure can be used for the shallow water equations: \( \mu' \), where \( d\mu' = \mathcal{D}[\eta] \mathcal{D}[h] \mathcal{D}[\mathbf{v}] \) with \( \eta = \delta h^3 \), \( \delta = \nabla \cdot \mathbf{v} \), is also an invariant measure. It can be proven by variable change [8]. The main advantage of this measure is that \( \eta \) is directly used as a microscopic variable.

We have justified the existence of two invariant measures over the phase space for the shallow water equations; we can now define the statistical mechanics of the system.
1.3.3 Microcanonical theory

In order to compute the statistical information on the system, we have to define the phase space $\Gamma$. As we study field statistical mechanics, we have an infinite-dimension phase space; in order to define the functions properly, we first discretize the phase space and take the continuous limit at the end. We will work with the measure $d\mu' = D[q]D[\eta]D[h]$.

Définitions We discretize the 2D domain into $N^2$ subdomains of equal area and denote $(q_{ij}, \eta_{ij}, h_{ij})$ the values of the fields at the point $(i,j)$. A given set $\{(q_{ij}, \eta_{ij}, h_{ij})\}_{i,j \in [1,N]}$, hereafter denoted $(q, \eta, h)^N$, is a microstate of the system in this phase space. We then define the microcanonical measure under $K$ constraints given by $K$ invariants $\{I_k(q, \eta, h)\}_{k \in [1,K]}$:

$$d\mu_N^2(\{I_k\}) = \frac{1}{\Omega_{N^2}^2} \prod_{i,j} dq_{ij} d\eta_{ij} dh_{ij} \prod_k \delta(I_k(q, \eta, h) - I_k^0)$$

(1.28)
where $\prod_{i,j} dq_{ij} d\eta_{ij} dh_{ij}$ is the discretized form of $D[q]D[\eta]D[h]$, and the normalization factor

$$\Omega_{N^2} = \int \prod_{i,j} dq_{ij} d\eta_{ij} dh_{ij} \prod_k \delta(I_k(q, \eta, h) - I_k^0)$$

(1.29)
is accessible phase space volume. Then the specific entropy can be defined following the Boltzmann formula, and the Boltzmann entropy of the continuous system is defined taking the continuous limit:

$$S(\{I_k\}) = \lim_{N \to \infty} \frac{1}{N^2} \log(\Omega_{N^2}(\{I_k\}))$$

(1.30)
which can be formally written

$$S(\{I_k\}) = \log \left( \int_{\mathcal{G}} \int_{\Gamma} D[q]D[\eta]D[h] \prod_k \delta(I_k(q, \eta, h) - I_k^0) \right).$$

(1.31)

For the shallow water equations the constraints are the conservation of energy and Casimirs, or equivalently the vorticity distribution, leading to:

$$S(E, D(\sigma)) = \log \left( \int_{\mathcal{G}} \int_{\Gamma} D[q]D[\eta]D[h] \delta(\sigma(q, \eta, h) - E) \int d\sigma \delta(D(q) - D(\sigma)) \right).$$

(1.32)

Alternative formulation and the Sanov theorem Directly computing the Boltzmann entropy is not possible for the Shallow water model, but an alternative method exists. Let us define a macrostate throught the local probablity $\rho(\mathbf{r}, q, \eta, h)$ to observe the microstate $(q, \eta, h)$ at $\mathbf{r}$. The mixing entropy is defined as:

$$\mathcal{S}[\rho] = - \int d\mathbf{r} \int dq d\eta dh \rho(\mathbf{r}, q, \eta, h) \ln \rho(\mathbf{r}, q, \eta, h).$$

(1.33)

If the system has a mean-field behavior, one can use the Sanov theorem to show that Boltzmann entropy $S$ is the maximum of $\mathcal{S}$ under the energy constraint $\mathcal{S}[h, \mathbf{v}] = E$, the vorticity distribution constraint (Casimirs) $D(\sigma)$, and the local normalization of the probability:

$$S(E, D(\sigma)) = \max_{\rho: N(\mathbf{r})=1} \{ \mathcal{S}[\rho] \mid D[q] = D(\sigma), \mathcal{S}[h, \mathbf{v}] = E_0 \}.$$ (1.34)

This mean-field behavior is well-known for Euler 2D (where the Casimirs strongly constrain the vorticity field). For the shallow water model, the $h$ field is constrained by the potential energy and thus obeys this mean-field behavior, but there is no guarantee that the divergent field follows the same rule. In the following, the computations will be done supposing this behavior, and this hypothesis will be tested numerically. Finding the system’s entropy is then a variational problem; we need to express the variations of the constrained quantities under a variation of macrostate $\delta \rho$. This is detailed in appendix A; here is the phase space volume, where $\bar{a}(\mathbf{r}) = \int d\mathbf{r} \rho(\mathbf{r}, q, \eta, h)a(\mathbf{r})$ is the coarse-grained field $a$, and $\beta$ is the inverse temperature:

$$\Omega(\mathbf{r}) = \int dq d\eta dh \exp \left\{ -h\alpha(q) - \beta \left( \frac{1}{2} \bar{h}^2 - hq\bar{\Psi}(\mathbf{r}) - h^{-3}\eta \bar{\Phi}(\mathbf{r}) + \frac{1}{2} gh^2 \right) \right\}$$

(1.35)
which gives access to the mean properties of the system:

\[ \bar{h}(\mathbf{r}) = -\int dq' \frac{\partial \ln \Omega}{\partial \alpha(q')} \]
\[ \bar{\omega}(\mathbf{r}) = \frac{1}{\beta} \frac{\partial \ln \Omega}{\partial \bar{\Psi}(\mathbf{r})} - f \]
\[ \bar{\delta}(\mathbf{r}) = \frac{1}{\beta} \frac{\partial \ln \Omega}{\partial \bar{\Phi}(\mathbf{r})} \]

These analytical results are not easy to use literally, so we turn to a numerical approach.

2 Sampling the microcanonical measure numerically

2.1 Definition of the algorithm

We shall now try to find a numerical algorithm that samples the accessible phase space with uniform distribution, under the energy and Casimirs constraints. One solution would be to create numerically random microstates and store them if they fit the constraints, but this wouldn’t be very efficient; instead we will use a Creutz algorithm.

Historically, the first algorithm of that kind was a sort of Monte-Carlo algorithm, the Metropolis-Hastings algorithm [5], which samples the canonical measure by creating a chain of microstates \( \{ s_n \}_{n \in \mathbb{N}} \) with probability \( ce^{-\beta H(q,p)} \).

Starting with a given microstate \( s_n = s \), the code tries a small random change on the microstate (hereafter called a move), leading to a new microstate \( s' \); then the algorithm accepts or rejects the move with a well-chosen probability. If the move is accepted, \( s' \) is stored as a new microstate \( s_{n+1} \) of the chain; if it is rejected, \( s_{n+1} = s \) is stored as the new state of the chain. The algorithm must be reversible, that is to say, the probability to try a move leading to \( s' \) starting from a microstate \( s \) is the same as the probability of trying a move to \( s \) starting from \( s' \). This ensures that the sampled distribution is the one we expect.

The Creutz’s algorithm [4] is a variant of the Metropolis-Hastings algorithm that can sample the microcanonical measure. The moves are designed to conserve most of the constraints (the Casimirs in the case of the shallow water equations) and to be reversible. They are accepted if the energy of the new state \( s' \) fulfills the energy constraint \( E - \delta E \leq E \leq E \), and rejected otherwise; this step in the algorithm will be denoted as the energy check. It has been used efficiently to sample the microcanonical measure of fluid systems described by the 2-dimensionnal Euler equations [6].

It is usual to define a Monte-Carlo time step as the number of moves which are necessary to affect each particle once on average. We shall define a Monte-Carlo time step more precisely after discussing the details of the moves in Sec.2.3.

Let us see how these ideas apply to a fluid described by the shallow water equations. In order to deal with the Casimirs constraint easily, one should use the microscopic variables \( (q, \eta, h) \) to describe the system (see Sec.1.3.1 for the definitions). In order to explore the entire phase space, we shall define different moves to mix properly the values of the fields \( q, \eta \) and \( h \) at any point \( \mathbf{r} \). We will see that four different moves are necessary to explore the whole accessible phase space.

2.2 Numerical system

2.2.1 Definition of the system

The numerical system we are studying is a fluid whose movement is described by the shallow water equations. This fluid evolves in a basin with area \( L \times L \) and mean height \( H \), under the action of the gravity field \( g \) and of the Coriolis force, described by the Coriolis parameter \( f \).

For simplicity’s sake, we shall work with a two-level potential vorticity distribution. The two available values for \( q \) will be denoted \( q_1 \) and \( q_2 \), so that \( D(\sigma) = \frac{1}{2} \delta(\sigma - q_1) - \frac{1}{2} \delta(\sigma - q_2) \), \( D(\sigma) \) being defined in Sec.1.2. Within this scheme, the conservation of the \( q \) distribution (which we recall to be equivalent to the conservation of all Casimirs) reduces to the conservation of the two “ occupied volumes ” defined as

\[ V_i = \int_{\mathcal{S}} d\mathbf{r} \bar{h}(\mathbf{r}) \delta(q(\mathbf{r}) - q_i) \]  

one for each possible value of \( q \).

We shall define the available energy as the energy over the minimal potential energy of the system, such as it reads:

\[ E_A = E - \frac{1}{2}gH^2 \]
We note that $E_A \geq 0$ and that $\min(E_A) = 0$.
The system is thus described by the 9 parameters $L, H, f, g, q_1, q_2, V_1, V_2$, and $E_A$. We have to decide how to fix these 9 parameters.

2.2.2 Dimensional analysis

First of all, let us choose the length and time units. The Coriolis parameter $f$ controls the typical time scale of geophysical phenomena, we will therefore use a time unit in which $f = 1$. A detailed dimensionnal analysis shows that the unit system for the vertical and horizontal dimensions can be chosen independently [7]; we will therefore use a length unit in which $L = 1$ for the horizontal dimension and a length unit in which $H = 1$ for the vertical dimension.

In geophysical studies, the flow is generally described with some dimensionless parameters; among them are two parameters of interest for us:

- the Rossby number compares the local vorticity of the flow with the global vorticity driven by the Coriolis force; it is generally written as $\epsilon = \frac{U}{fL}$, where $U$ is the order of magnitude of the velocity. Typical geophysical flows have small Rossby numbers, for it is the Coriolis force which dominates the movement. Moreover, a theorem called the Proudman-Taylor theorem shows that this importance of the Coriolis force leads to quasi 2-dimensionality in geophysical flows

- the Rossby radius of deformation is more easily interpreted in a multi-layer system: the different layers are separated by fronts which will be horizontal at rest, but may be deformed with the flow. The Rossby radius of deformation represents the typical spatial scale of the deformations of these fronts. This number is obviously related to the gravity field $g$ and is generally written as $L_R = \frac{1}{f} \sqrt{gH}$, or in terms of the Froude number $F = \frac{L}{L_R} \epsilon$

Of course $U$ is not a parameter of our simulation but an internal variable, so we must redefine these parameters, but we will use them as a template.

As we have six parameters remaining, we could first impose some others arbitrary constraints on the system. Let us choose a system with periodic boundaries; this creates a constraint on the values of $q_i$ and $V_i$:

$$\int_D \mathbf{dr} \cdot \mathbf{\omega} = 0 = \int_D \mathbf{dr} \cdot (q \mathbf{h} - f) \Rightarrow \int_D q_1 V_1 + q_2 V_2 = fL^2$$

(2.3)

In addition, if we arbitrarily fix $V_1 = V_2 = \frac{1}{2} HL^2$, the previous condition reduces to $q_1 + q_2 = 2 \frac{f}{H}$.

We thus have three constraints remaining; we will define three dimensionless parameters which describe the system:

$$\epsilon_e = \frac{1}{f} \sqrt{\frac{E_A}{H}}$$

(2.4)

$$\epsilon_v = \frac{(q_1 - q_2)H}{f}$$

(2.5)

$$F = \frac{L}{L_R} \epsilon_e$$

(2.6)

The first one is a Rossby number defined within the assumption that all the available energy is mainly kinetic energy (which is just a way to fix $E_A$ but does not imply that the system is effectively kinetic); $\epsilon_v$ is a Rossby number based on the potential vorticity values; $F$ is the usual Froude number with respect to $\epsilon_e$. In the numerical work, we shall use these three parameters as control parameters.

2.2.3 Grid definitions

Here we carefully choose the discretization grid for the spatial domain. The microscopic variables we work with are $(q, \eta, h)$, as it gives a simple way to manage Casimirs conservation. The drawback of this choice lies in the energy check step: in order to compute the new energy after a move, we have to recalculate the whole velocity field using either FFT or a laplacian inversion routine. Even though this is perfectly correct, it is numerically slow as both of these operations are numerically scaling as $N \ln N$, $N$ being the number of grid sites. We then tried to find a local algorithm, that is to say an algorithm in which each move only impacts a restricted number of grid sites, and in which it is possible to compute the energy check only on these few sites (this step then scaling as 1).

Even if the microcanonical problem is defined by the microscopic variables $(q, \eta, h)$, we shall then keep track of the velocity values during the moves; this allows us to compute a local energy check for most of the moves, as will be shown below (Sec.2.3). We insist on the fact that computing local energy checks is neither a physical nor a numerical
In order to keep track of both the sets of variables \( v_x, v_y \) on the one hand, and of \( q, \eta \) (which are easily related to the vorticity \( \omega = (\nabla \times \mathbf{v}) \cdot \mathbf{e}_z \) and to the divergence field \( \delta = \nabla \cdot \mathbf{v} \)) on the other hand, we need to define the grid so that simple relations can be written between the two sets. Since only two degrees of freedom are needed at each lattice point \((v_x, v_y)\) and \(\delta, \omega\), for example, we only need to consider the velocities as written on Fig. 2. We denote \((i, j)\) the position on the \(q\) lattice and \((i + \frac{1}{2}, j + \frac{1}{2})\) the corresponding position on the \(\eta\) lattice. Choosing this particular staggered grid allows for very natural definitions for the vorticity \(\omega\) and the horizontal divergence \(\delta\) with a finite-difference scheme:

\[
\omega_{i,j} = \frac{N}{L} \left( v^y_{i+\frac{1}{2},j} - v^y_{i-\frac{1}{2},j} + v^x_{i,j-\frac{1}{2}} - v^x_{i,j+\frac{1}{2}} \right) \tag{2.7}
\]

\[
\delta_{i+\frac{1}{2},j+\frac{1}{2}} = \frac{N}{L} \left( v^y_{i+\frac{1}{2},j+1} - v^y_{i+\frac{1}{2},j} + v^x_{i+1,j+\frac{1}{2}} - v^x_{i,j+\frac{1}{2}} \right). \tag{2.8}
\]

We recall that \(\eta = h^3 \delta, q = \frac{\omega_L}{h}\) and \(h\) define a microstate. The height \(h\) is labelled on the \((i, j)\) lattice. The energy per unit mass computation from the discrete fields then needs a prescription to be performed. We will use the definition:

\[
E_{kin} = \frac{L^2}{N^2} \sum_{i,j} \frac{1}{4} \{ (h_{i,j} + h_{i+1,j})(v^y_{i+\frac{1}{2},j})^2 + (h_{i,j} + h_{i,j+1})(v^x_{i,j+\frac{1}{2}})^2 \} \tag{2.9}
\]

\[
E_{pot} = \frac{L^2}{N^2} \sum_{i,j} \frac{1}{2} gh^3_{i,j}. \tag{2.10}
\]

Defining \(\eta\) also needs a prescription; we shall define

\[
\eta_{i+\frac{1}{2},j+\frac{1}{2}} = h^3_{i+\frac{1}{2},j+\frac{1}{2}} \delta_{i+\frac{1}{2},j+\frac{1}{2}} \quad \text{with} \quad h_{i+\frac{1}{2},j+\frac{1}{2}} = \frac{h_{i,j} + h_{i+1,j} + h_{i,j+1} + h_{i+1,j+1}}{4}. \tag{2.11}
\]

All these prescriptions are approximations, up to second-order corrections, of the continuous quantities and lead to the correct continuous limit when \(N \to \infty\).

This particular staggered grid matches all the necessities discussed above: we have simple relations between the speed components and the \((q, \eta)\) description. We shall now define the moves.

---

**Figure 2: Definition of the lattices**
2.3 Definition of the moves

A move must mix three quantities: \(q\) values, \(h\) values and \(\eta\) values. In addition, a fourth move will be added to mix the areas occupied by the vorticity levels, as will be explained in Sec. 2.3.1. These quantities must be mixed conserving the \(q\) values \(q_1\) and \(q_2\) and the volumes \(V_i\) at each step.

These different parts are described below. For each step, it is important to notice that the algorithm is reversible, that is to say, the probability of reaching a microstate \((q, \eta, h)^N\) starting from \((q, \eta, h)^N\) is the same as reaching \((q, \eta, h)^N\) starting from \((q, \eta, h)^N\). As explained above, this is a necessary condition (called the detailed balance condition) to sample the correct probability distribution (for detail, see [6], appendix A and B).

2.3.1 \(q\) move

The first move is designed to simply mix the \(q\) values on the lattice points:

1. a direction (vertical or horizontal) is randomly chosen with probability \(1/2\) for each. We describe here the horizontal permutation case, but generalization to vertical permutations is straightforward
2. a lattice site \((i, j)\) is randomly chosen; if \((i + 1, j)\) has the same \(q\) value, another site \((i, j)\) is chosen
3. we wish to swap both values of \(q\) and \(h\) between \((i, j)\) and \((i + 1, j)\); this move conserves the Casimirs, as can be easily seen from the volumes’ definition Eq.(2.1)

4. we now have to perform an energy check. This move has introduced a local change in the vorticity field:

\[
\omega_{i,j} \rightarrow \omega_{i,j} + h_{i+1,j}q_{i+1,j} - h_{i,j}q_{i,j}
\]

and

\[
\omega_{i+1,j} \rightarrow \omega_{i+1,j} + h_{i,j}q_{i,j} - h_{i+1,j}q_{i+1,j}.
\]

Instead of maintaining \(\eta\) and recalculating all the velocity field with FFT, we locally compensate the change in \(\omega\) by applying

\[
v_i^y \rightarrow v_i^y + \frac{1}{N}(h_{i+1,j}q_{i+1,j} - h_{i,j}q_{i,j}) = v_{i+\frac{1}{2},j}^y + \Delta v_{i+\frac{1}{2},j}^y.
\]

It is now possible to perform the energy check locally with

\[
\Delta E_{kin} = \frac{L^2}{N^2} \left\{ \frac{h_{i,j} + h_{i+1,j}}{4} \Delta v_{i+\frac{1}{2},j}^y (2v_{i+\frac{1}{2},j}^y + \Delta v_{i+\frac{1}{2},j}^y) \right\}.
\]

We note that the potential energy is conserved during this move.

5. if the move is accepted, then the \(q\) and \(h\) values are swapped, the velocity is updated and the \(\eta\) field is locally recalculated to take the \(v_{i+\frac{1}{2},j}^y\) modification into account.

First of all, we notice that the local computation of the energy difference is only possible because there is no physical constraint on the \(\eta\) field, allowing us to use it as an adjustment variable. This technique was inspired by ??.

Secondly, we check that the algorithm is reversible: the probability to pick the same direction and the same lattice point is always the same, and this would reverse the move.

Finally, this move is simple but has a default: it conserves not only the volumes \(V_i\), but also the areas occupied by the \(q\) levels, defined as \(A_i = \int_q dr \delta(q(r) - q_i)\). Since this is not a physical constraint, we shall define an additional move that mixes these areas; it will be discussed in Sec. 2.3.4

2.3.2 \(h\) move

1. a direction (vertical or horizontal) is randomly chosen with probability \(1/2\) for each; we describe here the horizontal permutation case, but generalization to vertical permutations is straightforward
2. a lattice point \((i, j)\) is randomly chosen; if \((i + 1, j)\) has a different \(q\) value, another site \((i, j)\) is chosen
3. an amount \(\Delta h\) is randomly chosen from a zero-mean gaussian distribution; as we have a straightforward constraint \(h > 0\) on the space domain, we have to reject any \(\Delta h\) making a \(h\) value negative. If, after this move, the same site is chosen with \(-\Delta h\), the move must be accepted as well (reversibility). In order to ensure that, we check if \(|\Delta h| < \min(h_{i,j}, h_{i+1,j})\), and choose another \(\Delta h\) otherwise. The variance of the distribution will be discussed at the end of the paragraph
4. if this condition is fulfilled, we perform \(h_{i,j} \rightarrow h_{i,j} + \Delta h\) and \(h_{i+1,j} \rightarrow h_{i+1,j} - \Delta h\). This move conserves the Casimirs, as can be easily seen from the volumes’ definition Eq.(2.1)
5. since the values of $q$ remain the same while the values of $h$ are modified, the vorticity values $\omega = qh - f$ are also modified: we locally update $v_{i+\frac{1}{2},j}^h \rightarrow v_{i+\frac{1}{2},j}^h + \frac{L}{N^2} q_{i,j} \Delta h = v_{i+\frac{1}{2},j}^h + \Delta v_{i+\frac{1}{2},j}^h$

6. perform the energy check:

$$\Delta E_{\text{kin}} = \frac{L^2}{N^2} \left\{ \frac{\Delta h}{4} \left( (v_{i-\frac{1}{2},j}^x)^2 + (v_{i-\frac{1}{2},j}^y)^2 + (v_{i+\frac{1}{2},j+\frac{1}{2}}^x)^2 + (v_{i+\frac{1}{2},j+\frac{1}{2}}^y)^2 - (v_{i+1,\frac{1}{2},j}^x)^2 - (v_{i+1,\frac{1}{2},j}^y)^2 - (v_{i+1,j+\frac{1}{2}}^x)^2 - (v_{i+1,j+\frac{1}{2}}^y)^2 \right) + \frac{h_{i,j} + h_{i+1,j}}{4} \Delta v_{i+\frac{1}{2},j}^y (2v_{i+\frac{1}{2},j}^y + \Delta v_{i+\frac{1}{2},j}^y) \right\},$$

(2.13)

and $E_{\text{pot}} = g \Delta h \{ \Delta h + (h_{i,j} - h_{i+1,j}) \}.$

(2.14)

7. if the move is accepted, then the $h$ values are modified by $\pm \Delta h$, and the velocity and the $\eta$ field are updated. The algorithm is reversible for the same reasons as the $q$ move, taking into account the condition on $\Delta h$ mentioned above.

The gaussian’s variance for $\Delta h$ must be chosen carefully. We notice that the potential energy $\frac{1}{2} g \int d\tau (h - H)^2$ is, up to a factor $g/2$, the variance of the $h$ distribution over the entire domain. It is then reasonable to choose the total energy as an upper bound for the standard deviation of the $\Delta h$ distribution. We finally choose a standard deviation $10^{-3}H$ for the simulations presented in Sec.3, in which the total available energy is 0.01.

### 2.3.3 $\eta$ move

1. a lattice site $(i + \frac{1}{2}, j + \frac{1}{2})$ is randomly chosen
2. an amount $\Delta \delta$ is randomly chosen from a zero-mean gaussian distribution and $\eta_{i+\frac{1}{2},j+\frac{1}{2}}$ is increased by $h_{i,j}^3 \Delta \delta$
3. in order to apply this change without changing the values of $\omega$, $v_{i+\frac{1}{2},j}^x$ and $v_{i+\frac{1}{2},j}^y$ are decreased by $\Delta v = \frac{L}{N^2} \frac{\Delta \delta}{4}$ and $v_{i+1,\frac{1}{2},j+\frac{1}{2}}^x$ and $v_{i+1,\frac{1}{2},j+\frac{1}{2}}^y$ are increased by $\Delta v$, so that each change in the four neighbouring $\omega$ lattice points are zero
4. the energy check is performed:

$$E_{\text{kin}} = \frac{L^2}{N^2} \Delta v \left\{ - \frac{h_{i,j} + h_{i+1,j}}{4} (2v_{i+\frac{1}{2},j}^y + \Delta v) - \frac{h_{i,j} + h_{i+1,j}}{4} (2v_{i+\frac{1}{2},j+\frac{1}{2}}^y + \Delta v) + \frac{h_{i,j} + h_{i+1,j}}{4} (2v_{i+\frac{1}{2},j+\frac{1}{2}}^x + \Delta v) + \frac{h_{i+1,j} + h_{i+1,j+1}}{4} (2v_{i+1,\frac{1}{2},j+\frac{1}{2}}^x + \Delta v) \right\}$$

(2.15)

as the potential energy is conserved during this move
5. if the move is accepted, the $\eta$ and velocity fields are updated.

The variance of the gaussian for $\Delta \delta$ is chosen such as a move roughly leads to $\Delta E \approx E_A/N^2$.

### 2.3.4 Area move

The first three moves conserve the areas occupied by each value of $q$; since this is not a physical constraint, we shall define a permutation step which mixes them. A first attempt was:

1. a lattice site $(i, j)$ is randomly chosen; it will be denoted 0 and its neighbours will be denoted by the subscripts $t, b, l, r$ (top, bottom, left, right), $n$ being the number of neighbours with the same $q$ value as 0
2. if $n \neq 4$, we check that $h_0/(4 - n) < \min(h_{\text{neighbours at } -q_0})$ in order to ensure reversibility and positive $h$ values
3. the $q$ value of 0 is switched: $q_0 \rightarrow q_0'$
4. in order to conserve the Casimirs, the height must be redistributed: the $n$ neighbours for which $q = q_0$ are changed according to $h \rightarrow h + \frac{h_0}{n}$ and the $4 - n$ others according to $h \rightarrow h - \frac{h_0}{4-n}$
5. the local change in $\omega$ is then compensated performing the proper modifications on $v_t, v_b, v_l, v_r$
6. the energy check is performed
7. the values of the $\eta$ lattice are updated
This does not work because the height variation is way too important. The second idea was then to use a well-sized \( n \times n \) subregion to redistribute the height field into smaller amounts, but the difficulty to recalculate the \( v \) field arose. Three possibilities were considered:

- local inversion of the Laplacian: it is not possible to impose a zero value for the velocity variation at the borders while imposing nonzero-values for the \( q \) variation at the borders, due to the discretization scheme and the used routine (from the fortran library fishpack)
- the same scheme has been examined on a subdomain of 1 per \( N \) lattice points, but this leads to a non-invertible matrix.
- writing a linear system on the equations:

\[
\begin{align*}
\text{n}^2 \text{ on the vorticity:} & \quad -\Delta v_{i,j+1/2}^x + \Delta v_{i+1,j}^y + \Delta v_{i,j-1}^x - \Delta v_{i-1,j}^y = (L/N)\Delta \omega \\
2n \text{ for the borders, for example:} & \quad \Delta v_{i+1/2,n-1}^y = 0 \\
\text{the rest on the divergence:} & \quad -\Delta v_{i,j+1/2}^x - \Delta v_{i+1/2,j}^y + \Delta v_{i+1,j+1/2}^x + \Delta v_{i+1/2,j+1}^y = 0
\end{align*}
\] (2.16)

but this also leads to a non-invertible matrix.

Finally, it has been decided to use a slower algorithm, working at the global scale:

1. a lattice site \((i,j)\) is randomly chosen, and will be denoted with the subscript 0; \( n \) is the number of sites on the field with the same value for \( q \)
2. if \( h_{i,j}/(N^2 - n - 1) \) is smaller than the minimal \( h \) value (ensuring reversibility), the algorithm can continue
3. the \( q \) value of \((i,j)\) is switched to the other possible value: \( q_0 \rightarrow q_0' \)
4. in order to conserve the Casimirs, the height must be redistributed; the \( n \) sites for which \( q = q_0 \) are changed according to \( h \rightarrow h + \frac{h_0}{N} \) and the \( N^2 - n - 1 \) others according to \( h \rightarrow h - \frac{h_0}{N^2 - n - 1} \); this reequilibrates the volumes, as can be easily seen from the volumes definition Eq.(2.1)
5. the new velocity array is computed by laplacian inversion using fortran library fishpack
6. the energy check is performed

This algorithm scales as \( O(N^2 \ln(N)) \); in order to keep the global algorithm quick, this permutation step is performed only \( N \) times while the others are performed \( N^2 \) times; this amount of permutations will be used as a definition for a Monte Carlo time step.

### 2.4 Temperature computation using the Creutz algorithm

We show here how one can compute numerically the inverse temperature from the energy distribution at equilibrium. We know that \( \frac{1}{N^2} \log \Omega_{N^2}(E) \xrightarrow{N \rightarrow \infty} S(E) \). In the same limit, the entropy has a well-defined peak at equilibrium. Using a Taylor expansion, we write \( S(E) \simeq S(E_0) + \beta(E - E_0) \), where \( \beta = \frac{dS}{dE}(E_0) \) is defined as the inverse temperature. We therefor have the relation:

\[
\ln \Omega_{N^2} \simeq S_{N^2}(E_0) + \beta N^2(E - E_0).
\] (2.17)

A histogram of the energy samples \( \Omega_{N^2} \) up to a normalization factor. We can then compute \( \beta \) for each \( E_0 \) by creating a histogram of the energy and measuring the slope of the logarithmic histogram.

### 3 First results

In this part we present the results of the first Monte-Carlo runs. These have been performed with a \( 64 \times 64 \) grid. As values of geophysical interest for the Rossby number are around 0.1, we shall use it as a starting point for our investigations. We first set both of our definitions of the Rossby number (Eq.(2.4)) to 0.1. In order to see large-scale structure appear eventually at scale \( L \), we set the Rossby deformation radius at \( L \), or equivalently the Froude number at 0.1. In the second simulation, we tried to give more importance to the vortical part of the kinetic energy by setting \( \epsilon_v = 1.0 \) while keeping the other parameters constant. Finally, we tried to enhance the gravity field’s action by setting \( \epsilon_e, \epsilon_v = 0.1 \) and \( F = 0.5 \).
### 3.1 Energy distribution

#### 3.1.1 First run: $\epsilon_e = \epsilon_v = 0.1, F = 0.1$

The energy properties of the system during the simulation are shown on Fig.3.

![Energy evolution during the simulation](image1)

(a) Energy evolution during the simulation

![Zoom on the energy](image2)

(b) Zoom on the energy

![Vortical kinetic energy part in total kinetic energy](image3)

(c) Vortical kinetic energy part in total kinetic energy

![Inverse temperature computation](image4)

(d) Inverse temperature computation

Figure 3: Energy evolution and repartition: $\epsilon_e = \epsilon_v = 0.1, F = 0.1$

First of all, Fig.3a shows that the warming time for our algorithm is about 10,000 Monte-Carlo time steps; we will therefore only store the microstates after the 40,000 first Monte-Carlo time steps to compute statistical properties. Fig.3b gives a general overview of the energy distribution: microstates with a higher energy are more numerous, leading to a clearly positive temperature. Fig.3c shows that the amount of vortical energy in the kinetic energy is small. Finally, Fig.3d shows that the energy distribution is compatible with a temperature value of 160, according to the method explained in Sec.2.4.

Since Fig.3a seems to show an equipartition between two kinetic degrees of freedom ($M_x$ ans $M_y$) and one spatial degree of freedom ($h$), one can compute the statistical properties assuming that the Casimirs’ constraints have little influence on the statistics. Under this assumption, the Hamiltonian of the system is, in the $(M_x, M_y, \delta h)$ coordinates (where $\delta h = h - H$):

$$H(M, \delta h) = \sum_{i=1}^{N^2} \frac{1}{2} g \delta h_i^2 + \frac{1}{2} \frac{M_{x,i}^2 + M_{y,i}^2}{H + \delta h_i}$$

Then the canonical partition function can be computed:

$$Z = \int_{-H}^{\infty} \prod_{i=1}^{N^2} d\delta h_i \int_{-\infty}^{\infty} \prod_{i=1}^{N^2} dM_x, dM_y, d\epsilon e^{-\frac{1}{2} \sum_{i=1}^{N^2} (g \delta h_i^2 + \frac{M_{x,i}^2}{H + \delta h_i} + \frac{M_{y,i}^2}{H + \delta h_i})}$$

$$= \left\{ \frac{2\pi}{\beta} \right\}^{3/2} \frac{H}{\sqrt{g}} \right \}^{N^2}$$

(3.2)

where we approximated $\int_{-H}^{\infty} \delta h_i$ with $\int_{-\infty}^{\infty} \delta h_i$ (this can be justified by the fact that the potential energy $\frac{1}{2} g \int_{h}^{\infty} dr (h - H)^2$ is, up to a factor $g/2$, the variance of the $h$ distribution over the entire domain, and then $|h - H| \ll H$).
Within this simple model, one can show that an equipartition theorem holds, so that:

\[ E = \frac{3}{2\beta} \Rightarrow \beta = 150 \]  \hfill (3.3)

This is approximately the inverse temperature computed as the entropy derivative on Fig.3d. As this seems to be a correct approximation, we will study the statistics of the \( h \) field in Sec.3.2.

### 3.1.2 Second run: \( \epsilon_e = 0.1, \epsilon_v = 1.0, F = 0.1 \)

The energy evolution of the system during the simulation is given on Fig.4. The remarks of Sec.3.1.1 also apply to this run, with some minor changes. First of all, we see that the equipartition no longer works, and that the results are compatible with \( \beta = 112 \), which means that the temperature increased. We also note that the vortical part of the kinetic energy increased, which is normal since we increased the values of the potential vorticity, but the kinetic energy still remains largely dominated by the divergent energy.

### 3.1.3 Third run: \( \epsilon_e = \epsilon_v = 0.1, F = 0.5 \)

The energy evolution of the system during the simulation is given on Fig.5. In this run, the gravitation field is 25 times weaker than precedently, every other parameter being the same as in the first run. The immediate consequence we can see in Fig.5a is that the potential energy strongly decreases, destroying the equipartition. The temperature strongly increased in this run, as can be seen from the computation of \( \beta = 83 \) in Fig.5d, and from the global shape of the fluctuations on Fig.5b. The ratio between vortical and divergent part of the kinetic energy is almost the same as in the first run, which seems natural since we did not change the parameters directly related to the Casimirs.
Figure 5: Energy evolution and repartition: $\epsilon_e = \epsilon_v = 0.1, F = 0.5$

### 3.2 $h$ field analysis

#### 3.2.1 First run: $\epsilon_e = \epsilon_v = 0.1, F = 0.1$

The probability for the $h$ field at site $j$ to be at the value $H + \delta h$ is:

$$P_j(\delta h) = \frac{1}{Z} \int_{-\infty}^{\infty} \prod_{s=1}^{N^2} dM_{x,s} dM_{y,s} \prod_{k \neq j} d\delta h_k e^{-\frac{1}{2} \beta \sum_{s,k} (g\delta h^2_k + \frac{M_{x,s}^2 + M_{y,s}^2}{M_{x,s}^2 + M_{y,s}^2})} e^{-\frac{1}{2} \beta g \delta h^2 + \sum_{s} \frac{M_{x,s}^2 + M_{y,s}^2}{M_{x,s}^2 + M_{y,s}^2}} = \sqrt{\frac{\beta g}{2\pi}} \left(1 + \frac{\delta h}{H}\right) e^{-\frac{1}{2} \beta g \delta h^2}$$

We can fit a histogram of the $h$ field (created from the values of the $h$ field in 9 different microstates) in order to have a new estimate for $\beta$. The result is shown on Fig.6.

We can see on these fits that our description is compatible with the results, even if the gaussian distribution seems to be even more accurate than the distribution Eq.(3.4). A possible explanation is that the approximation $\int_{-\infty}^{\infty} \approx \int_{-\infty}^{\infty}$ would be compensated by the approximation $1 + \frac{\delta h}{H} \approx 1$ leading to a more accurate gaussian description.

#### 3.2.2 Second run: $\epsilon_e = 0.1, \epsilon_v = 1.0, F = 0.1$

The histogram of the $h$ field and the fits with $\beta = 112$ are shown on Fig.7. The remarks of Sec.3.2.1 also apply to this run.
3.2.3 Third run: $\epsilon_e = \epsilon_v = 0.1, F = 0.5$

The histogram of the $h$ field and the fits with $\beta = 83$ are shown on Fig.8. The remarks of Sec.3.2.1 also apply to this run.
3.3 Absence of large-scale structures

Let us look at the map of averaged streamfunctions $\Psi$ and $\Phi$ and to their typical values.

3.3.1 First run: $\epsilon_e = \epsilon_v = 0.1, F = 0.1$

![Figure 9: $\Psi$ maps and distribution: $\epsilon_e = \epsilon_v = 0.1, F = 0.1$](image)

![Figure 10: $\Phi$ maps and distribution: $\epsilon_e = \epsilon_v = 0.1, F = 0.1$](image)

It is clear from Fig.10 that the values of $\Phi$ are randomly distributed over the map; this is not surprising, as $\Phi$ is related to the divergent part of the field, which is not constrained by the Casimirs.

The global shape of Fig.9a seems to show a large-scale structuration of the $\Psi$ streamfunction, but since the $\Psi$ field does not seem to follow the same pattern in the microstates (Fig.9b), a more precise analysis is needed. Because the fluctuations of the $\Psi$ field (shown on the field distribution Fig.9b) are much larger than the average values on the map Fig.9a, we cannot conclude that such structures exist over a long period of time. A more precise analysis would be necessary to reach proper conclusion regarding the existence of such structures (for example by recording a histogram of $h$ for each lattice site), but we did not have enough time to do it during this internship.

These results are why, in the next simulations, we first tried to enhance the importance of the Casimirs (we worked with more important values of the potential vorticity by increasing the Rossby number based on the vorticity $\epsilon_v$) in order to make such large-scale structures appear; then we tried to see if the equipartition description holds with a weaker gravitation field in the third run.
3.3.2 Second run: $\epsilon_c = 0.1, \epsilon_v = 1.0, F = 0.1$

Fig.11 and Fig.12 show the maps for the $\Psi$ and $\Phi$. The remarks made in Sec.3.3.1 apply to this run: even if large-scale structures seem to appear on Fig.11a, they don’t seem to be persistent enough. For lack of time, we did not try higher values for $\epsilon_v$.

![Figure 11: $\Psi$ maps: $\epsilon_c = 0.1, \epsilon_v = 1.0, F = 0.1$](image)

3.3.3 Third run: $\epsilon_c = \epsilon_v = 0.1, F = 0.5$

Fig.13 and Fig.14 show the maps for the $\Psi$ and $\Phi$. The same remarks as Sec.3.3.1 apply: even if large-scale structures seem to appear on Fig.13a, they don’t seem to be persistent enough.
Conclusion

The statistical mechanics of the shallow water model is a very complex subject. We showed how the theory can be constructed and why it is not possible to extract direct information analytically. We described the algorithm that was constructed and coded during the internship, even though there were many technical problems during the development. The few first results obtained with this code do not show clear large-scale vortical structures as we expected, but present a very fluctuating height field (similar to the simulation shown on the wikipedia page on the shallow water equations). This was expected: there is no constraint on the divergence field, which is directly related to the height field.

We will complete this study by running the working code with different parameter values, and try to understand the statistical behavior of the shallow water equations.
A Canonical theory

A.1 Constraints

The constraint on the energy is not straightforward to write down; let us write the energy:

$$E[h,v] = \frac{1}{2} \int dr (hv^2 + gh^2). \quad (A.1)$$

It would be convenient to write this quantity as a function of the macrostate, that is to say as a function of mean fields $\bar{h} = \int \rho(q,\eta,h)h dr$ and $\bar{v} = \int \rho(q,\eta,h)v dr$. Since the velocity can be written in terms of the $\omega$ and $\delta$ fields using Green functions:

$$v = \int \mathcal{D}r' \bar{G}_\omega(r,r')\omega(r') + \int \mathcal{D}r' \bar{G}_\delta(r,r')\delta(r') \quad (A.2)$$

and since $\omega$ and $\delta$ are not long-range correlated, there is no long-range correlation in the velocity field. Therefore the kinetic part can be re-written $\frac{1}{2} \int \bar{h}\bar{v}^2 dr$.

The potential part is more complicated, as there is no reason to consider $\bar{h}^2 = \bar{h}^2$; in other words, there is no reason to consider an absence of long-range correlations. Nevertheless, the formula (1.33) for the mixing entropy supposes no long-range interaction; therefore, it will be consistent to suppose $\bar{h}^2 = \bar{h}^2$. Finally, the energy variation can be written:

$$\delta E = \int dr \int dq d\eta dh \left\{ \frac{1}{2} \bar{h}^2 - \bar{q} h + \frac{1}{2} g \bar{h}^2 \right\} \delta \rho(r,q,\eta,h). \quad (A.3)$$

The constraint on the Casimirs will be written as the conservation of the occupied volume $V(q)$ by any given value of $q$:

$$V(q) = \int dr \int d\eta dh \rho(r,q,\eta,h) \rightarrow \delta V(q) = \int dr \int d\eta dh \delta \rho(r,q,\eta,h). \quad (A.4)$$

The normalization constraint says that the probability function $\rho$ is normalized at each point $r$:

$$N(r) = \int dq d\eta dh \rho(r,q,\eta,h) = 1 \Rightarrow \delta N(r) = \int dq d\eta dh \delta \rho(r,q,\eta,h). \quad (A.5)$$

A.2 Solution of the variational problem

Let us introduce the Lagrange parameters $\beta$ (energy constraint), $\alpha(q)$ (Casimirs) and $\lambda(r)$ (normalization); the variational problem then reads

$$\delta S - \beta \delta E - \int dq d\eta dh \rho(r,q,\eta,h) \delta \bigg( V(q) \bigg) = 0 \quad (A.6)$$

which leads to:

$$\rho(r,q,\eta,h) = \frac{1}{\Omega(r)} \exp \left\{ -h\alpha(q) - \beta \left( \frac{1}{2} \bar{h}^2 - \bar{q} h - \bar{h}^{-3} \eta \bar{h} + \frac{1}{2} g \bar{h}^2 \right) \right\} \quad (A.7)$$

where

$$\Omega(r) = \int dq d\eta dh \exp \left\{ -h\alpha(q) - \beta \left( \frac{1}{2} \bar{h}^2 - \bar{q} h - \bar{h}^{-3} \eta \bar{h} + \frac{1}{2} g \bar{h}^2 \right) \right\}. \quad (A.8)$$

This partition function gives access to the mean properties of the system:

$$\bar{h}(r) = -\int dq \frac{\partial \ln Z}{\partial \alpha(q')} \quad (A.9)$$

$$\bar{\omega}(r) = \frac{1}{\beta} \frac{\partial \ln Z}{\partial \Psi(r)} - f$$

$$\bar{\mu}(r) = \frac{1}{\beta} \frac{\partial \ln Z}{\partial \Phi(r)}$$
References


