Some numerical methods for a maximum entropy problem

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Abstract. We describe a numerical method developed to treat the statistical equilibrium model of coherent structures in two-dimensional turbulence. We explain the statistical model for which the method was designed to solve. A convergence proof is given along with several alternative methods for the same problem. The solution of this problem requires maximizing a nonlinear functional subject to nonlinear constraints.

1. Introduction

The equations which describe two-dimensional inviscid fluid flow are the Euler equations. As time evolves these flows become highly chaotic and turbulent on increasingly smaller and smaller spatial scales. Traditional numerical methods applied to this time dependent problem are limited by the requirement of resolving these small scales. Recently, a statistical theory for the equilibrium solution of these equations has been proposed using methods from statistical mechanics. This statistical equilibrium solution for the Euler equations is obtained by maximizing a nonlinear functional characterizing an entropy subject to the natural constraints of the flow. One of the constraints is also nonlinear making this a nontrivial optimization problem. In [**8**] and [**9**], we develop an accurate and highly efficient iterative algorithm for solving this optimization problem. If one attacked this optimization problem in the usual way numerically, an enormous system would have to be solved at each iterate and there is no guarantee that the algorithm would converge. By exploiting the structure of the optimization problem, we are able to solve a simple nonlinear problem at each iterative step. We prove that our algorithm converges globally. In [**8**] and [**9**], we demonstrate the correctness of the statistical theory along with some failings by comparing our results with numerical results from traditional methods applied to the time dependent problem. We observe such classical phenomenon as the rollup of periodic vortex layers and the merger of patches of vorticity.

In this paper, we explain the method given in [**8**] along with 2 other methods proposed for the first time here. This paper is organized as follows. In section 2, we give the equations describing the flow of a viscous incompressible fluid, the Navier-Stokes equations. In section 3, we show how the Euler equations, which describe the flow of an inviscid, incompressible fluid, are obtained. In section 4, we give the

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conserved quantities of the flow. In section 5, we explain the statistical theory of Miller-Robert which predicts the most probable flow to the Euler equations and associates this flow with the equilibrium solution. In section 6, we present our numerical method to solve the problem formulated by the statistical theory. In section 7, we present an equivalent simple dual problem which we actually solve. In section 8, we discuss the convergence proof for the algorithm and in section 9, we present other algorithms given for the first time.

2. Navier-Stokes Equations

The two-dimensional flow of an incompressible fluid is described by the Navier-Stokes equations

$$\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} + \nabla p = \nu \triangle \vec{v}, \tag{2.1}$$

$$\frac{\partial v_1(\vec{x},t)}{\partial x_1} + \frac{\partial v_2(\vec{x},t)}{\partial x_2} = 0. \tag{2.2}$$

where $\vec{v} = (v_1(\vec{x},t), v_2(\vec{x},t))$ and $p = p(\vec{x},t)$ are the velocity and pressure fields and $\nabla = (\partial/\partial x_1, \partial/\partial x_2)$ with $\vec{x} = (x_1, x_2)$. The viscosity is given by ν and $\triangle$ is the standard Laplacian. These equations hold within a domain $\Omega \subseteq R^2$, with the boundary condition $n \cdot \vec{v} = 0$ imposed on $\partial\Omega$, where n denotes the outward unit normal field. It is widely recognized now, from both the theoretical and computational points of view, that the salient features of this fluid dynamics are more concisely described by the vorticity field $\omega(\vec{x},t)$ defined by

$$\omega(\vec{x},t) = \frac{\partial v_2}{\partial x_1} - \frac{\partial v_1}{\partial x_2} \tag{2.3}$$

Incompressiblity (2.2) implies that there exists a streamfunction $\psi(\vec{x},t)$ such that,

$$\vec{v} = \left(\frac{\partial \psi}{\partial x_2}, -\frac{\partial \psi}{\partial x_1}\right).$$

and combining that with (2.3) above, we have that

$$\omega(\vec{x},t) = -\frac{\partial^2 \psi}{\partial x_1 x_1} - \frac{\partial^2 \psi}{\partial x_2 x_2} = - \triangle \psi(\vec{x},t)$$

Equation (2.1) can be written in terms of the vorticity and velocity only and is given by

$$\frac{\partial \omega(\vec{x},t)}{\partial t} + \vec{v} \cdot \nabla \omega(\vec{x},t) = \nu \triangle \omega(\vec{x},t) \tag{2.4}$$

$$\omega(\vec{x},0) = \omega_0(\vec{x}) \tag{2.5}$$

$$\psi = 0 \text{ on } \partial\Omega \tag{2.6}$$

instead of the primitive fields $\vec{v}$ and p.

Equation (2.4) describes the transport of the vorticity. Numerically, these equations are difficult of solve especially for a small viscosity ν. As the viscosity decreases, smaller scales become more and more important and a finer grid is needed to approximate the equations numerically. For a reasonable viscosity, one can easily overwhelm the most powerful computers.

3. Euler Equations

For $\nu = 0$, equations (2.4)-(2.6) become the Euler Equations,

$$\frac{\partial \omega(\vec{x},t)}{\partial t} + \vec{v} \cdot \nabla \omega(\vec{x},t) = 0. \tag{3.1}$$

$$\omega(\vec{x},0) = \omega_0(\vec{x})$$

$$\psi = 0 \text{ on } \partial\Omega$$

with

$$\omega(\vec{x},t) = - \triangle\, \psi(\vec{x},t)$$

These equations are almost impossible to solve numerically because of the infinitely small scales involved, nevertheless, they have a simple interpretation. Given a vorticity particle trajectory $(t, \vec{x}(t))$, equation (3.1) can be written as

$$\frac{d\omega(\vec{x}(t),t)}{dt} = 0.$$

The means that the value of the vorticity is just transported along particle paths, i.e., $\omega(\vec{x},t)$ is just a rearrangement of $\omega(\vec{x},0)$ for $t > 0$. In our presentation, we consider only so-called vortex patches, i.e., $\omega(\vec{x},0) = 0$ or $\omega(\vec{x},0) = 1$. Consequently, as time goes on the vorticity $\omega(\vec{x},t)$ takes on the same values 0 and 1. However $\mid \nabla\omega(\vec{x},t) \mid$ grows rapidly in t, such that the patches develop smaller and smaller scale fluctuations. Any numerical method is limited by the higher and higher resolution required as time goes on.

4. Conserved Quantities

Certain quantities are invariant in the flow. The initial circulation Γ_0 at time 0 is given by,

$$\Gamma_0 = \int_\Omega \omega(\vec{x},0) d\vec{x}$$

and the initial energy E_0 at time 0 is given by,

$$E_0 = \frac{1}{2} \int_\Omega \omega(\vec{x},0)\psi(\vec{x},0) d\vec{x}.$$

As ω evolves, the circulation Γ and the energy E are conserved for all time, i.e.,

$$\Gamma = \int_\Omega \omega(\vec{x},t) d\vec{x} = \Gamma_0$$

and

$$E = \frac{1}{2} \int_\Omega \omega(\vec{x},t)\psi(\vec{x},t) d\vec{x} = E_0.$$

This can be verified by differentiating the quantities E and Γ with respect to time and using the differential equation. There are other conserved quantities depending on the geometry of Ω. In [**9**], we find the equilibrium solution in a disk, which has the additional conserved quantity

$$M = \int_\Omega \omega(\vec{x},t) \frac{|\vec{x}|}{2} d\vec{x}.$$

In [8], we find the equilibrium solution in a x_1-periodic domain with dirichlet boundary conditions in x_2. Here,

$$I = \int_\Omega \omega(\vec{x}, t) x_2 d\vec{x}.$$

is also conserved.

5. Miller-Robert Theory

The Euler equations are difficult to solve therefore we will try to use some ideas from statistical mechanics. Suppose that we start with some initial flow or initial vorticity $\omega_0(\vec{x})$ and wish to find the equilibrium vorticity distribution. Let the

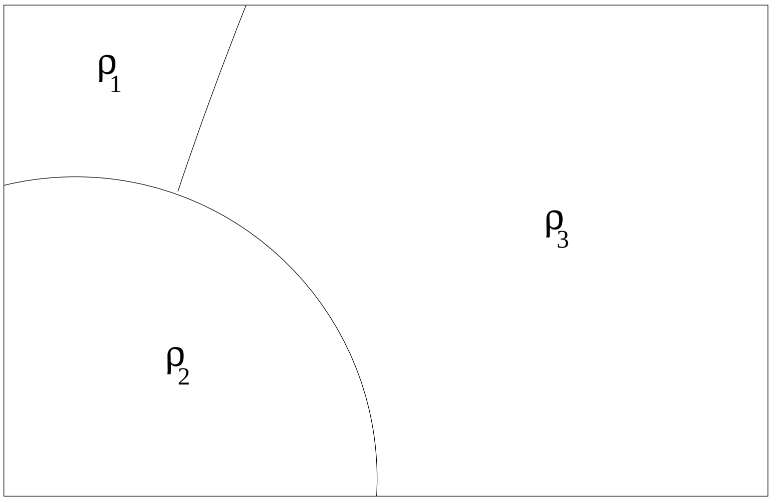

FIGURE 1. This represents all possible microstates partitioned.

region in figure 1 represent all the vorticity functions with the same circulation and energy of our given vorticity function $\omega_0(\vec{x})$. These admissible functions represent microscopic variables. We attempt to partition and associate with a subset of microscopic variables, a macroscopic variable $\rho(\vec{x})$. In figure 1, for the purpose of clarity, we assume there are only 3 possible macroscopic variables. Based on figure 1, we might guess that our equilibrium solution lies in the class described by $\rho_3(\vec{x})$. We now explain the partitioning strategy given proposed by Miller and Robert in a series of papers([2], [3], [4], [5]). We attempt to find the macroscopic variable which contains the most microscopic variables. We then hypothesize that most probably our equilibrium solution lies in this class. Robert argues that the macrostate which contains the most microstates contains overwhelmingly more than any other.

We give a heuristic derivation of the Miller-Robert theory which connects the microstates to the macrostates. We suppose that our domain Ω contains only 2 points X_1 and X_2 divided into N equal parts each where ω is 0 or 1 on each part.

Figure 2 gives a possible microstate. If we think of it's macrostate ρ as representing the local volume fraction at each point, then it is given by

$$\rho(X_1) = \frac{4}{9}, \ \ \rho(X_2) = \frac{5}{9}$$

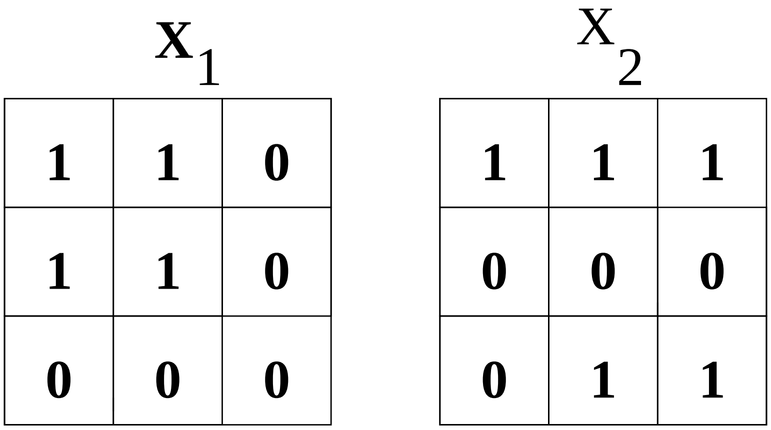

FIGURE 2. This represents our domain with 2 points.

which contains the microstate in figure 2. In fact, ρ contains

$$\frac{9!}{4!(9-4)!}\,\frac{9!}{3!(9-3)!}$$

microstates. If $\rho(X_1) = \frac{N_1}{N}$ and $\rho(X_2) = \frac{N_2}{N}$ then the number of microstates contained by this macrostate is

$$W(\rho) = \frac{N!}{N_1!(N-N_1)!}\,\frac{N!}{N_2!(N-N_2)!}.$$

Note also that $\rho(\vec{x})$ can be thought of as the probability that ω takes on the value 1 at $\vec{x}$. For our domain Ω the number of microstates associated with a macrostate is given by

$$W(\rho) = \prod_i \frac{N!}{N_i!(N-N_i)!}$$

where this product is taken over all the points in Ω. After some simplification, one finds that the macrostate ρ with the most microstates is the one which maximizes

$$S(\rho) = -\int_\Omega \rho\log(\rho) + (1-\rho)\log(1-\rho)d\vec{x}.$$

We can relate our macroscopic variable back to our microscopic variables. The expected value of the vorticity is given by

$$\bar{\omega}(x) = \rho(\vec{x})\cdot 1 = \rho(\vec{x})$$

should also satisfy the constraints:

$$\Gamma(\rho) = \int_\Omega \rho(\vec{x})d\vec{x} = \Gamma_0,$$

$$E(\rho) = \frac{1}{2}\int_\Omega \rho(\vec{x})\psi(\vec{x})d\vec{x} = E_0$$

where

$$\triangle\psi(\vec{x}) = -\rho(\vec{x}).$$

For example, suppose that we have a so-called shear layer as shown in figure 3 as

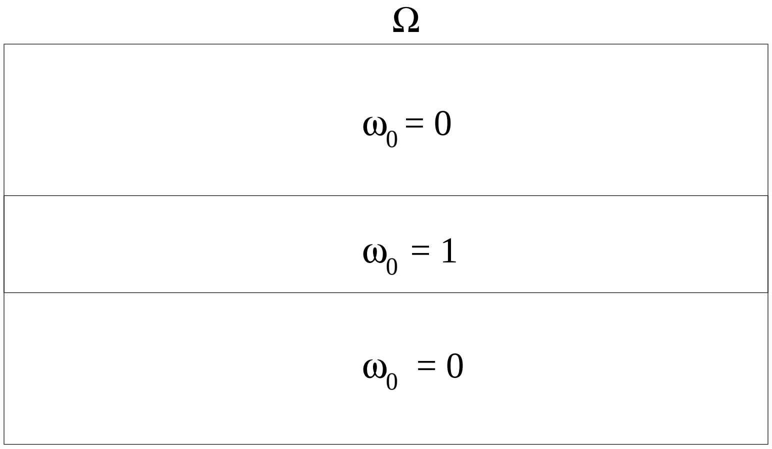

FIGURE 3. This represents initial data given by a shear layer.

our initial flow $\omega_0(\vec{x})$ and we wish to find the most probable solution which we will guess to be the long time solution. We first compute Γ_0 and E_0 associated with figure 3. Given Γ_0 and E_0 from above, we maximize

$$S(\rho) = -\int_\Omega \rho \log(\rho) + (1-\rho)\log(1-\rho) d\vec{x}$$

subject to

$$\Gamma(\rho) = \int_\Omega \rho d\vec{x} = \Gamma_0$$

and

$$E(\rho) = \frac{1}{2}\int_\Omega \rho\psi d\vec{x} = E_0$$

where

$$\triangle\psi(\vec{x}) = -\rho(\vec{x}).$$

There exists α and β by the Lagrange multiplier rule such that

$$S'(\rho) = \alpha\Gamma'(\rho) + \beta E'(\rho)$$

where in general $F'(\rho)$ denotes a functional derivative defined by

$$F(\rho + \delta\rho) = F(\rho) + < F'(\rho), \delta\rho > + o(\| \delta\rho \|).$$

For our equation, we have

$$S'(\rho) = -\log\frac{\rho}{1-\rho}$$

$$\Gamma'(\rho) = 1$$

$$E'(\rho) = \psi.$$

This implies

$$\rho = \frac{\exp(-\alpha - \beta\psi)}{1 + \exp(-\alpha - \beta\psi)} = -\triangle\psi. \tag{5.1}$$

It is also worth noting that

$$S''(\rho) = -\frac{1}{\rho(1-\rho)} < 0,$$

i.e., S is strictly concave.

6. Numerical Method

We now present our numerical method. In our numerical method, we compute ρ^{k+1} from ρ^k by solving the subproblem

$$S(\rho) \to \max, \text{ subject to} \tag{6.1}$$

$$\Gamma(\rho) = \Gamma_0, \tag{6.2}$$

$$E(\rho^k) + \int_\Omega E'(\rho^k)(\rho - \rho^k) d\vec{x} \geq E_0. \tag{6.3}$$

S is strictly concave and all the constraints are linear, therefore, the iteration produces a well-defined sequence then if ρ^0 satisfies $\Gamma(\rho^0) = \Gamma_0$ and $E(\rho^0) \geq 0$. The solution ρ^{k+1} satisfies

$$S'(\rho^{k+1}) = \alpha^{k+1}\Gamma'(\rho^{k+1}) + \beta^{k+1}E'(\rho^k).$$

$$\beta^{k+1} \leq 0,$$

$$\beta^{k+1}[E(\rho^k) + < E'(\rho^k), \rho^{k+1} - \rho^k > -E_0] = 0.$$

These are the Kuhn-Tucker conditions, a generalization of the Lagrange multiplier rule for inequalities([**1**],[**7**]). The above conditions imply that if $\beta^{k+1} \neq 0$, the inequality constraint holds with equality. The notation $< \cdot, \cdot >$ denotes the L^2 pairing. In a similar way as (5.1), one can solve for ρ^{k+1} to obtain,

$$\rho^{k+1} = \frac{\exp\left(-\alpha^{k+1} - \beta^{k+1}\psi^k\right)}{1 + \exp\left(-\alpha^{k+1} - \beta^{k+1}\psi^k\right)} \tag{6.4}$$

The right hand side contains two unknowns α^{k+1} and β^{k+1}. These can be solved uniquely by firstly integrating equation (6.4) and forcing it to satisfy the circulation constraint, equation (6.2) and secondly integrating equation (6.4) and forcing it to satisfy the linear energy constraint (6.3) with equality. This gives 2 nonlinear equations in 2 unknowns at each step with a unique solution. These equations are given by

$$\int_\Omega \rho^{k+1}(\vec{x}) d\vec{x} = \Gamma_0 \tag{6.5}$$

$$\int_\Omega \rho^{k+1}(\vec{x})\psi^k(\vec{x}) d\vec{x} = E_0 + E^k \tag{6.6}$$

This is a very inexpensive method. We solve the above system by a damped Newton's method. We calculate the integrals in (6.5) and (6.6) numerically using bicubic splines.

7. Dual Problem

The linearized problem (6.1), (6.2) and (6.3) which we solve at each step involves maximizing a functional defined at a huge number of points. In terms of the Lagrange multiplier rule it can be interpreted as follows. Let

$$G(\rho,\alpha,\beta) = S(\rho) - \alpha(\Gamma(\rho) - \Gamma_0) - \beta(E(\rho^k) + < E'(\rho^k), \rho - \rho^k > - E_0).$$

In solving the linearized problem, we find α^{k+1}, β^{k+1} and ρ^{k+1} such that

$$G(\rho^{k+1},\alpha^{k+1},\beta^{k+1}) \geq G(\rho,\alpha,\beta)$$

for every ρ in our admissible class and for all α and $\beta \leq 0$.

There is an associated dual problem which is equivalent to the above problem but results in solving a small system at each step. Minimize $\phi(\alpha,\beta)$ where

$$\phi(\alpha,\beta) = \alpha\Gamma_0 + \beta(E_0 + E(\rho^k)) + \int_\Omega \log(1 + \exp(\alpha + \beta\psi^k))d\vec{x} \tag{7.1}$$

with $\alpha \in R$ and $\beta \leq 0$. Minimizing (7.1) is equivalent to solving (6.5) and (6.6).

8. Convergence of the Numerical Method for $\beta < 0$

In section 4, we show that S is strictly concave. This leads to

$$S(\rho + \delta\rho) \leq S(\rho) + < S'(\rho), \delta\rho > -2 \parallel \delta\rho \parallel^2,$$

and using that E is convex, we have

$$E(\rho + \delta\rho) \geq E(\rho) + < E'(\rho), \delta\rho > .$$

By the convexity of E and the inequality constraint (6.3), we have

$$E(\rho^k) \geq E(\rho^{k-1}) + < E'(\rho^{k-1}), \rho^k - \rho^{k-1} > \ \geq E_0.$$

With a little manipulation, we arrive at the principle inequality for our convergence proof,

$$S(\rho^{k+1}) - S(\rho^k) \geq 2 \parallel \rho^{k+1} - \rho^k \parallel^2 + \beta^{k+1}[E_0 - E(\rho^k)]. \tag{8.1}$$

We see that if $\beta < 0$, the entropy increases along the iterative sequence and converges to some limit S^* as $k \to \infty$. We can then conclude that $E(\rho^k) \to E_0$ and that $\rho^{k+1} - \rho^k \to 0$ in L^2. This does not imply convergence of ρ^k which one would not expect due to the nonuniqueness of critical points. However, it is shown in [**8**] that the minimum distance between ρ^k and the set of critical points tends to zero as $k \to \infty$. The algorithm then converges for $\beta < 0$ only. Below, we give a new algorithm which works for positive β along with an alternative algorithm for negative β.

9. Other Algorithms

Another algorithm which we propose for negative β again is based on expanding the entropy to linear terms only and satisfying the energy constraint exactly at each iteration. The solution ρ^{k+1} is given by solving the subproblem,

$$\tilde{S}(\rho) \ \to \ \max \quad \text{subject to}$$

$$\Gamma(\rho) = \Gamma_0, \tag{9.1}$$

$$E(\rho) = E_0 \tag{9.2}$$

where

$$\tilde{S}(\rho) = \int_D S(\rho^k) + S'(\rho^k)(\rho - \rho^k) d\vec{x}$$

We have linearized the entropy above. Using the calculus of variations, we have the variational equation

$$S'(\rho^k) = \beta^{k+1}\psi^{k+1} + \alpha^{k+1}.$$

ρ^{k+1} is obtained uniquely by solving a linear system at each step. We have immediately,

$$\psi^{k+1} = \frac{S'(\rho^k)}{\beta^{k+1}} - \alpha^{k+1}$$

and

$$\rho^{k+1} = -\Delta\left(\frac{S'(\rho^k)}{\beta^{k+1}}\right)$$

The constant β^{k+1} is then determined by enforcing the circulation constraint(9.1) giving ρ^{k+1}. The multiplier α^{k+1} and ψ^{k+1} are determined by enforcing the energy constraint(9.2). The convergence proof is similar to those in the above algorithm but with a few modifications. Global convergence for $\beta \leq 0$ follows easily from the previous algorithm. Stability must be investigated however for this algorithm.

The algorithms presented above can be proven to work only if $\beta < 0$. We have recently developed an algorithm which can be applied to problems which have solutions corresponding to positive β. The principal inequality in the convergence proofs above is given by (8.1). If $\beta^{k+1} > 0$, then the proof will fail as outlined above unless $E(\rho^k) - E_0 \leq 0$. We can achieve this by solving our linearized maximum entropy problem with our previous iterate ρ^k to get an intermediate solution $\tilde{\rho}^{k+1}$ and obtain the corresponding streamfunction $\tilde{\psi}^{k+1}$. We then solve the following problem for ρ^{k+1}.

$$S(\rho) \rightarrow \max \quad \text{subject to}$$

$$\Gamma(\rho) = \Gamma_0,$$

$$E(\rho^k) + \int_D \tilde{\psi}^{k+1}(\rho - \rho^k) dx \leq E_0.$$

Two problems must be resolved at each step, however, it appears that this code exhibits a faster rate of convergence than the methods presented before. Another method for this problem is given also by [**6**].

References

[1] A.D. Ioffe and V.M. Tihomirov. *Theory of extremal problems.* Elsevier North-Holland, 1979.

[2] J. Miller. Statistical mechanics of Euler equations in two dimensions. *Phys. Rev. Lett.*, 65:2137, 1990.

[3] J. Miller, P. Weichman, and M.C. Cross. Statistical mechanics, Euler's equations, and Jupiter's red spot. *Phys. Rev. A*, 45:2328, 1992.

[4] R. Robert. A maximum-entropy principle for two-dimensional perfect fluid dynamics. *J. Stat. Phys.*, 65:531, 1991.

[5] R. Robert and J. Sommeria. Statistical equilibrium states for two-dimensional flows. *J. Fluid Mech.*, 229:291, 1991.

[6] R. Robert and J. Sommeria. Relaxation towards a statistical equilibrium state in two-dimensional perfect fluid dynamics. *Phys. Rev. Lett.*, 69:2776, 1992.

[7] R.T. Rockafellar. *Convex analysis.* Princeton Univ. Press, Princeton, N.J., 1970.
[8] B. Turkington and N. Whitaker. Statistical equilibrium computations of coherent structures in turbulent shear layers. *SIAM J. Comput.*, 17:1414, 1996.
[9] N. Whitaker and B. Turkington. Maximum entropy states for rotating vortex patches. *Phys. Fluids A*, 6:3963, 1994.

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