A Review of *STATISTICAL EQUILIBRIUM COMPUTATIONS OF COHERENT STRUCTURES IN TURBULENT SHEAR LAYERS* by BRUCE TURKINGTON AND NATHANIEL WHITAKER [1]

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Overview

Despite seeming like more of a physical science topic, the field of fluid dynamics is so ingrained with mathematics, that one of its outstanding questions, "Are there solutions to the Navier-Stokes Equations, and are they unique?" was named one of the Millennial prize problems. Thus, as is very evident, questions in fluid dynamics is as much a mathematical question as they are physical ones. However, for many of the question in fluid dynamics it is still not known whether solutions exist or not and despite that fact, numerical evaluation, even with some error, are still extremely valuable information to know when engineering planes, boats, and much more, or even in striving to reduce the drag on a triathlete or cyclist to give them an advantage over their competitors. Since this information can be so valuable, and with the advent of faster and faster computational machinery, much research in the mathematics of fluid dynamics is conducted using computer simulations to give approximate solutions to the aforementioned equation, or like in this paper, computational solutions to two dimensional statistical equilibrium problems. In order to solve this problem Turkington and Whitaker impose conditions on determining functions of the system in order to derive a couple simplifying results which they later use to prove both normal convergence for a system with specific, special, initial condition and the weak convergence of the general initial state of the system. After proving convergence they lay out the process for which the algorithm was numerically implemented to both maximize entropy and calculate sheer layers. Finally, they give specific plots that illustrated their points and expand on what those plots mean.

Key Terms

Statistical Equilibrium Problems-Problems, usually in statistical mechanics and mathematical physics which often refer to systems made up of a large number of, ideally independent, bodies which may or may not interact with each other. The equilibrium refers to the system being in its most probable macrostate based on the total number of microstates corresponding to that specific macrostate.
Vorticity Dynamics-The study of the movement of regions of fluid for which the primary competent of motion is rotation about an axis. Often the study of the pseudo vector field

$$\omega = \bigtriangledown \times \vec{u}$$

called the vorticity of the system in which $\vec{u}$ is the flow velocity.
Entropy-A measure of the multiplicity of the system, defined as

$$S(\Omega) = k_{Boltz} \ln \Omega$$

in which k_{boltz} is Boltzmann's constant, and Ω is the multiplicity, or simply the number of microstates of a system corresponding to a given macrostate. For example roll two ordinary dice, D_1 and D_2 and sum the numbers you get. For a macrostate of $D_1 + D_2 = 7$ the multiplicity is $\Omega = 6$ since there are 6 different possible ways to roll two dice and have their sum be 7. For larger and larger N, the multiplicity extraordinarily larger for the moderate values of macro state compared to the extremes, so much so that the second law of Thermodynamics is that Entropy tends to increase, or simply systems like to be in the state with the highest multiplicity because it is so much more probable.
Maximum Entropy State-Given the definition of Entropy above it is evident that the Maximum entropy states corresponds to the macrostate with the highest multiplicity.
Reynolds Number-Introduced by George Gabriel Stokes, the Reynolds number is a number used to predict similar flow pasterns in different fluid flow situations.
Shear Layer-a region of flow defined by a significant velocity gradient. Two common types include Boundary shear layers which arise from fluid passing over a solid boundary, and Free shear layers.
Free Shear Layer-In contrast to a boundary shear layers, Free shear layers occur without a sold object, but rather arise from structures within the fluid flow, for example between free flow and the wake of an object, but not the object itself.
Objective Function-It is either a loss function (to be minimized) or its negative, called a gain function (to be maximized) which associates events, or values to a real number corresponding to the cost or reward of that event.
Constrain Function-Simply a function which defines the parameters for which to optimize the objective function on.
Enstrophy-A potential density directly related to the Kinetic energy of the

fluid. Defined as the integral square of the vorticity

$$\mathcal{E}(\boldsymbol{\omega}) \equiv \frac{1}{2}\int_S \boldsymbol{\omega}^2 dS.$$

A similar definition exists in terms of flow velocity.
Bifurcation-Simply a division into two parts. With respect to mathematics, it refers to when a small change in parameters results in an evident change in the behavior of the output.
Roll-up Phenomenon-The rolling up of a fluid as it flows past a surface, often interpreted as turbulence, and often a low pressure zone.
Rate of Convergence-Simply characterized as the speed at which a convergent sequence approaches its limit. Defined as

$$\mu = \lim_{k\to\infty} \frac{|x_{k+1} - L|}{|x_k - L|}.$$

For $0 \leq \mu \leq 1$ the sequence is said to converge sub-linearly, and for $\mu > 1$ we say the sequence converges super-linearly.
Conjugate Functions-Defined as

$$f^*(y) = \sup_{x \in dom f} (y^T - f(x))$$

has the property that f^* is closed and convex even if f is not.
Stream function-Used to find the volumetric flux through a line connecting two points by finding the difference in the value of the Stream function between these two points. It is defined as

$$\psi = \int_A^P (u\,\mathrm{d}y - v\,\mathrm{d}x)$$

where we define u and v as follows

$$u = +\frac{\partial\psi}{\partial y} \quad \text{and} \quad v = -\frac{\partial\psi}{\partial x}.$$

For this specific application we have

$$\psi(x) = G\omega(x) = \int_D g(x,x')\omega(x')\mathrm{d}x'$$

in which G is the Green operator and $g(x,x')$ is the corresponding Green function.
Green Function-An integral kernel, much like the Poisson kernel, that is used to solve differential equations of the form $L[u(x)] = f(x)$ in which L is a linear differential operator. The solutions are of the form

$$u(x) = \int G(x,s)f(s)\mathrm{d}s.$$

High points

Turkington and Whitaker begin with a discussion on Vorticity dynamic in which convert the Euler equations in terms of velocity and pressure fields,

$$\frac{\partial v}{\partial t} + v \cdot \bigtriangledown v + \bigtriangledown p = 0, \quad \bigtriangledown \cdot v = 0$$

into one equation in terms of vorticity ω given by

$$\frac{\partial \omega}{\partial t} + v \cdot \bigtriangledown \omega = 0.$$

Finally, since the vorticity ω is related to the stream function by $\omega = - \bigtriangleup \psi$ they simply applied Green's operator to solve the system

$$\psi(x) = G\omega(x) = \int_D g(x, x')\omega(x')\mathrm{d}x'.$$

Turkington and Whitaker then outline one of the guiding principle from which they proceed. They lay out the Maximum entropy Principle which states that any system will tend towards it state of maximum entropy, a consequence of basic probability and thermodynamics. However, in order to answer this question by maximizing the Entropy $S(p)$, they acknowledge specific constraint imposed upon the system. The two major constraints imposed on the system are that the energy,

$$E(p) = \frac{1}{2}\int_D \bar{\omega} G \bar{\omega} \mathrm{d}x,$$

is constant and the enstrophy,

$$F(p; f) = \int_D \mathrm{d}x \int_l f(y)p(x, \mathrm{d}y),$$

is independent of the particular macrostate for which the system finds itself. In a more symbolic and concise form, simply that

$$S(p) \to \max \quad \text{subject to} \quad E(p) = E_0, \quad \text{and} \quad F(p; f) = F_0(f).$$

Shortly after defining and deriving terms, Turkington and Whitaker mention that both these constraints can be derived from the initial vorticity field ω_0. Then, they begin to explain their process for maximizing the entropy based on different somewhat simplifying implication of the constraints they imposed on the original problem. First off, Turkington and Whitaker are able to conclude that the mean flow in equilibrium for this problem satisfies semi-linear elliptic equation,

$$- \bigtriangleup \bar{\psi} = \Phi'(\bar{\psi} \quad \text{with} \quad \Phi(s) = -\beta^{-1} \log \int_l \exp(-\alpha(y) - \beta y s)p_0(\mathrm{d}y).$$

In which $\alpha(y)$ and β are completely determined by the constraints on $E(p)$ and $F(p; f)$ through an eigenvalue eigenvector problem and thus are also completely determined by the initial vorticity field ω_0. However, the equations described above imply that the statistical equilibrium problem can possibly have multiple solutions each with bifurcating solution branches, making a direct solution extremely difficult. However, the Maximum entropy principle as they initially stated it admits various extensions under the constrained imposed on it, each of which corresponds to a symmetry in the domain geometry and flow configuration. Now, since there are apparent symmetries there must also be corresponding conserved quantities. Note though, since this paper aimed to answer question about sheer layers, they focus on the conserved quantity associated with those structures. Hence, they state that the x_1 component of linear impulse,

$$M = \int_D x_2 \omega dx$$

is in fact that conserved quantity allowing for the simplifying substitution

$$M(\rho) = M_0.$$

After exploring the advantages they receive by imposing the condition that $E(p) = E_0$ and $F(p; f) = F_0(f)$ Turkington and Whitaker then proceed to explore some of the other implications that these constraints impose on the system. The first of which is that since they are hold $E(p)$ constant, there is a range of values $[E_{min}, E_{max}]$ such that their previous approximations are feasible. They proceed find what these values are by through simple optimization processes than with can be applied to the entropy. For example, to find E_{max} they solved the constrained maximization problem

$$E(\omega) \to \max \quad \text{subject to} \quad C(\omega) = C_0, \quad 0 \leq \omega \leq \lambda$$

thus giving them definitive upper and lower bounds on the Energy and Enstrophy of the system. From this, they know that the energy of the system in its most common macrostate ρ_{hom}, and thus maximum entropy is given by $E_{min} < E(\rho_{hom}) < E_{max}$. From this they outline some characteristics that the system holds in the real world, but that may not necessarily hold in more complex geometries.

After these comparisons the authors begin their exposition of the iterative algorithm they use to find computational solution to the originally stated problem. Their iterative step generates the vorticity field step ω^{k+1} from the previous step ω^k by solving the optimization problem obtained by linearizing the energy function,

$$\int_D \omega G \omega^k \mathrm{d}x \to \quad \max \quad \text{over} \quad C(\omega) = C_0, \quad 0 \leq \omega \leq \lambda.$$

Which is designed to be globally convergent, meaning that it converges for any initial vorticity field, ω_0. This can be concluded from the inequality

$$E(\omega^{k+1}) - E(\omega^k) \geq E(\omega^{k+1} - \omega^k).$$

Following this exposition, the authors begin their section regarding the a numerical iterative algorithm to an approximate solution of the maximum entropy problem initially stated. They use the work of the previous section to help define the iterative step, however for this problem, they iterate over the macrostates, ρ in such that the total Entropy is maximized,

$$S(\rho) \to \max \quad \text{subject to} \quad C(\rho) = C_0, \quad E(\rho^k) + \langle E'(\rho^k), \rho - \rho^k \rangle \geq E_0$$

which we know converge whenever the initial macrostate ρ^0 satisfies the conditions

$$C(\rho^0) = C_0 \quad \text{and} \quad E(\rho^0) \geq E_0.$$

Curiously, we also find that the solutions satisfy the Kuhn-Tucker Conditions,

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

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

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

where $\alpha^{k+1}, \beta^{k+1} \in \mathbf{R}$ serve as a natural extension of the Lagrange multipliers for inequality constrained problems. In addition we learn that the solution triplet generated, $(\rho^{k+1}, \alpha^{k+1}, \beta^{k+1})$, is determined completely by those condition when combined with the initial constraints on the problem. Finally, Turkington and Whitaker begin their discussion on the convergence properties of the iterative algorithm they just defined, including a proof of convergence of their numerical iterative algorithm, the details of which can be found in the following section. Additionally, they found that their algorithm converged at a linear rate to an isolated, but not unique solution. An astoundingly fast rate of convergence in computational methods. After proving the convergence of the algorithm, they expound upon the numerical implementation of the iterative algorithm. In their numerical implementation of the iterative algorithm, in order to reduce the computational burden, they simply ignore the inequality constraint on β and the problem becomes a system of nonlinear equations

$$\left(\frac{\partial}{\partial \alpha}, \frac{\partial}{\partial \beta}, \frac{\partial}{\partial \gamma} \right) \int_D s^*(\alpha\gamma + \beta\lambda\bar{\psi}^k(x) + \gamma\lambda x_2) \mathrm{d}x = (C_0, E_0 + E^k, M_0)$$

in which we see our invariant M_0 coming into play. This equation is then solved using a Damped Newton method with dampening factor of $2^- m$, where m is taken to be the smallest nonnegative integer for which the residual is decreased in the Euclidean norm, to ensure convergence. They also define the stopping criterion they used to get their rate of convergence as

$$\frac{||\rho^{k+1} - \rho^k||}{||\rho^k||}, \frac{||S^{k+1} - S^k||}{||S^k||}, \frac{||E^{k+1} - E^0||}{||E^0||} \leq 5 \times 10^{-3}.$$

Finally, they touch vaguely upon the typical number of iteration for the algorithm's computation of shear layers to converge, as well as the specification and justification for the typical grid size and number of points to evaluate the model based on rate of convergence and on accuracy of solution.

Key Proof

Convergence of Iterative Algorithm to a Solution of Maximum Entropy Problem

Turkington and Whitaker first expand both the energy function and entropy function to second order

$$S(\rho + \delta\rho) \leq S(\rho) + \langle S'(\rho), \delta\rho\rangle - 2||\delta_\rho||^2,$$

$$E(\rho + \delta\rho) = E(\rho) + \langle E'(\rho), \delta\rho\rangle + 2E(\delta_\rho).$$

Along with the initial Kuhn-Tucker condition, they derived the fact that

$$S(\rho^{k+1}) - S(\rho^k) - 2||\rho^{k+1} - \rho^k||^2 \geq \langle S'(\rho^{k+1}), \rho^{k+1} - \rho^k\rangle$$

$$\langle S'(\rho^{k+1}), \rho^{k+1} - \rho^k\rangle = \beta^{k+1}\langle E'(\rho^k), \rho^{k+1} - \rho^k\rangle$$

$$\beta^{k+1}\langle E'(\rho^k), \rho^{k+1} - \rho^k\rangle = \beta^{k+1}[E_0 - E(\rho^k)]$$

and hence they have that

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

Now, they point out that the terms involving α^{k+1} vanish because C is a linear functional, and that by the convexity of E we know that,

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

Hence, they derived the inequality

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

which is true for all k and arbitrarily admissible ρ^0. Thus, it is evident that the entropy increases with each iteration, which in combination with the fact that by definition, the entropy is bounded, Turkington and Whitaker conclude that the algorithm must converge to a finite value. Now, they proceed to prove that the limit is actually a solution to the stated problem. From the monotonicity of $S(\rho^k)$ it must be that $\rho^{k+1} - \rho^k \to 0$ in L^2 and hence the sequence ρ^k must then also converge to a limit ρ^*. Now, since we know that $\rho^k \to \rho^*$ in L^2 as $k \to \infty$ it is relatively trivial to see from the previous sections that both corresponding multipliers, α^k and β^k must converge to α^* and β^* respectively. Therefore, the triplet $(\rho^*, \alpha^*, \beta^*)$ solves the equation for statistical equilibrium

$$S'(\rho^*) = \alpha^* C'(\rho*) + \beta^* E'(\rho^*).$$

They then go on to show that under weakened constraints, $C(\rho^*) = C_0$, and $E(\rho^*) \geq E_0$ that

$$C(\rho + \epsilon\eta) = C_0,$$

$$E(\rho^k) + \langle E'(\rho^k), \rho + \epsilon\eta - \rho^k\rangle \geq E(\rho^*) + \langle E'(\rho^*), \rho - \rho^*\rangle - \epsilon_k + \epsilon$$

and hence that

$$E(\rho^k) + \langle E'(\rho^k), \rho + \epsilon\eta - \rho^k \rangle \geq E_0 - \epsilon_k + \epsilon.$$

Therefore, by defining Σ^* to be the set of critical points ρ^* of the maximum entropy problem, they have shown that by taking $k \to \infty$

$$dist_G(\rho^k, \Sigma^*) := \inf_{\rho^* \in \Sigma^*} ||\rho^k - \rho^*|| \to 0$$

where the G norm is defined as

$$||\rho_G^2 = \int_D \rho G \rho \mathrm{d}x.$$

Hence, they show that the previously defined iterative algorithm is globally convergent to a solution of the Maximum Entropy Problem.

Reference

1. B. Turkington, and N. Whitaker, Statistical Equalibrium Computation of Coherent Structures In Turbulent Shear Layers, SIAM J. ScI. COMPUT., **Vol. 17, No. 6** (November 1996), 1414-1433.