ANALYSIS OF MODEL VARIANCE FOR ENSEMBLE BASED TURBULENCE MODELING

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Abstract. This report develops an ensemble or statistical eddy viscosity model. The model is parameterized by an ensemble of solutions of an ensemble-Leray regularization. The combined approach of ensemble time stepping and ensemble eddy viscosity modeling allows direct parametrization of the turbulent viscosity coefficient that gives an unconditionally stable algorithm. We prove that the model's solution approaches statistical equilibrium as $t \to \infty$; the model's variance $\to 0$ as $t \to \infty$. The ensemble method is used to interrogate a rotating flow, testing its predictability by computing effective averaged Lyapunov exponents.

Key words. ensemble, Leray regularization, eddy viscosity, turbulence modeling

1. Introduction. The goal of conventional turbulence models (CTMs) is to produce a model that accurately predicts time averaged or ensemble averaged flow statistics. Thus a CTM should quickly converge (in time) to statistical equilibrium that captures averaged flow behavior. This differs from large eddy simulation models that seek to represent the essentially dynamic behavior of local spacial averages. The problem addressed herein is how to give an analytic theory for "convergence to statistical equilibrium" of models and algorithms. We develop a new family of turbulence models herein and study their convergence by analyzing the evolution of model variance.

Let $\langle \cdot \rangle$ denote an ensemble average. The conventional/RANS turbulence model (from the ensemble averaged Navier-Stokes equations (NSE)) for $\langle u \rangle$ is

$$\begin{gathered}\langle u\rangle_t + \langle u\rangle\cdot\nabla\langle u\rangle - \nabla\cdot([\nu+\nu_T(l,k')]\nabla\langle u\rangle) + \nabla\langle q\rangle = \langle f\rangle\,,\text{ in }\Omega, \\ \nabla\cdot\langle u\rangle = 0, \langle u\rangle(x,0) = \left\langle u_j^0\right\rangle(x)\text{ in }\Omega\text{ and }\langle u\rangle = 0\text{ on }\partial\Omega.\end{gathered} \tag{1.1}$$

In (1.1), the eddy viscosity (EV) term[1] $\nabla\cdot(\nu_T(l,k')\nabla\langle u\rangle)$ replaces the divergence of the Reynolds stresses

$$\begin{gathered}\text{Reynolds stress: } R(u,u) := \langle u\rangle\langle u\rangle - \langle uu\rangle\,, \\ -\nabla\cdot R(u,u) \quad\text{replaced by }\; -\nabla\cdot(\nu_T(l,k')\nabla\langle u\rangle)\,.\end{gathered}$$

Since (1.1) is a model, its solution is no longer the exact ensemble average. The turbulent viscosity coefficient is given by the Kolmogorov-Prandtl relation

$$\begin{gathered}\nu_T(l,k') = Const.l\sqrt{k'}, \\ k' = \text{ kinetic energy in fluctuations,} \\ l\ = \text{mixing length.}\end{gathered}$$

The unknowns k', l are often modeled by solving additional systems of nonlinear PDEs. On the other hand, if eddy viscosity models are fundamentally sound and if k' can be directly calculated, without modeling, then using an exact value for k' must increase the physical fidelity of (1.1).

Calculating k' requires solving an ensemble of NSE realizations. New algorithms for ensemble simulation (began in [19]) put this within reach (and possibly at lower cost than modeling k').

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[1] Since $\nabla\cdot\langle u\rangle = 0$, this form with the full gradient of $\langle u\rangle$ is equivalent to one with deformation tensor.

When k' can be directly calculated, ν_T can be directly calculated giving an ensemble eddy viscosity model. Ensemble eddy viscosity was studied as a numerical regularization in [19], [17]. Interestingly, its use as a numerical regularization leads to the wrong system for $\langle u \rangle$ (not (1.1)). This report shows that ensemble simulation of (1.1) requires new realization equations including

$$u_{j,t} + \langle u \rangle \cdot \nabla u_j - \nabla \cdot ([\nu + \nu_T(l, k')]\nabla u_j) + \nabla p_j = f_j(x,t) \text{ and } \nabla \cdot u_j = 0, \tag{1.2}$$

derived in Section 3. (1.2) contains sufficient regularizations to make its solution plausibly less expensive than a full DNS for each realization. Further, time discretizations of (4.1), (4.6) are unconditionally stable. In the methods (4.1), (4.6) below, each time step requires the solutions of J linear systems with a shared coefficient matrix reducing both storage and work

$$A \left[\begin{array}{c|c|c} u_1 & \cdots & u_J \\ p_1 & \cdots & p_J \end{array} \right] = \left[RHS_1 \,|\cdots|\, RHS_J \right], \tag{1.3}$$

by use of direct methods, projective, [10], or block iterative methods, e.g., [25], [11], [1], [9], [12].

Section 4 presents two numerical methods for (1.2) that allow these efficiencies. These are proven unconditionally, nonlinearly, long time stable. For example, for (1.2) the following linearly implicit-explicit backward Euler method has these favorable features. With superscript denoting the time step number, (and suppressing spacial discretization) for $j = 1, ..., J$

$$\begin{aligned} &\frac{u_j^{n+1} - u_j^n}{\Delta t} + \langle u \rangle^n \cdot \nabla u_j^{n+1} + \nabla p_j^{n+1} \\ -\nu \Delta u_j^{n+1} &- \nabla \cdot (2\nu_T(l^n, k'^n)\nabla^s u_j^{n+1}) = f_j^{n+1}. \end{aligned} \tag{1.4}$$

We prove that the variance of (1.4) converges to zero as $t^n \to \infty$. In other words, the solution of (1.4) converges to statistical equilibrium as $t^n \to \infty$. This is the first result of this kind we are aware of.

A second order accurate extension with linear system structure (1.3) is given in Section 4 where unconditional stability is proven. Section 2 introduces the definition of variance and its evolution equation. An important consequence (a proof of the Boussinesq assumption) is discussed. Section 3 gives the derivation of (1.2) and three other models. Section 5 gives a few numerical tests for $2d$ forced turbulence. These quantify the difference between the solution of the model herein and the method studied in [19]. The averaged, effective Lyapunov exponent is also calculated to verify that ensemble Leray regularization is effective to squeeze two trajectories together (Proposition 3.2).

1.1. Previous Work. Incomplete data, quantification of uncertainty and sensitivities and other issues, e.g., [4], [14], [20], [23], [24], [26], require simulation of flow ensembles. This leads to the competition between ensembles vs. high resolution [15]. In [18] a new algorithm addressing this competition was given.

The number of ensemble members J can often be taken moderate. The "bred vectors" algorithm of Toth and Kalnay [26] gives a small set of perturbations of initial conditions (thus a small ensemble size) that capture maximal ensemble spread. In [32], an interesting paper studying statistical ensemble of large eddy simulations, it is found that 16 realizations suffice to provide reliable statistics and the results change little for more realizations. With J small, ensemble simulation becomes competitive with approaches based on solving auxiliary systems of PDEs for the turbulent parameterizations in (1.1).

This approach to ensemble parametrization was begun in [19] where the mixing length $l = |u'|\triangle t$ was investigated. However in [19], EV is a numerical regularization and not a true turbulence model. The ensemble based parametrization (herein) connects the method to ideas and diagnostics from the statistical theory of turbulence, [2], [6], [7], [8].

2. Variance evolution in the Navier-Stokes equations. One goal in a CTM is to achieve a statistically steady solution, i.e., one with variance = 0. Before analyzing model variance, we present the behavior of the Reynolds stresses and the evolution of variance for the Navier-Stokes equations. Consider the $2d$ or $3d$ NSE where the ensemble is generated by a distribution of initial conditions

$$\begin{aligned} &u_{j,t} + u_j \cdot \nabla u_j - \nu \triangle u_j + \nabla p_j = f(x,t), \text{ in } \Omega,\ j = 1, ..., J, \\ &\nabla \cdot u_j = 0, \text{ and } u_j(x,0) = u_j^0(x), \text{ in } \Omega \text{ and } u_j = 0, \text{ on } \partial\Omega. \end{aligned} \tag{2.1}$$

We assume that all solutions are strong solutions.

Definition 2.1 (Variance). *The variance of u and ∇u are*

$$V(u) := \left\langle ||u_j||^2 \right\rangle - || \left\langle u_j \right\rangle ||^2 \textit{ and } V(\nabla u) := \left\langle ||\nabla u_j||^2 \right\rangle - || \left\langle \nabla u_j \right\rangle ||^2.$$

Recall the (standard) result that variance measures fluctuations.

Lemma 2.2. *We have*

$$V(u) = \left\langle ||u_j'||^2 \right\rangle \geq 0 \textit{ and } V(\nabla u) = \left\langle ||\nabla u_j'||^2 \right\rangle \geq 0.$$

Proof. This is a standard calculation. Insert $u_j = \langle u_j \rangle + u_j'$ and expand each term. ∎

Averaging the ensemble NSE gives the equation for ensemble averages, $\nabla \cdot \langle u \rangle = 0$ and

$$\begin{gathered} \langle u \rangle_t + \langle u \rangle \cdot \nabla \langle u \rangle - \nu \triangle \langle u \rangle + \nabla \langle p \rangle - \nabla \cdot R(u,u) = f(x,t), \\ \text{where } R(u,u) := \langle u \rangle \langle u \rangle - \langle uu \rangle . \end{gathered}$$

Since all solutions are strong solutions we may calculate the kinetic energy in the mean flow by taking the inner product with $\langle u \rangle$. This gives

$$\frac{1}{2}\frac{d}{dt}|| \langle u \rangle ||^2 + \nu||\nabla \langle u \rangle ||^2 + \int_\Omega R(u,u) : \langle u \rangle \, dx = \int_\Omega f(x,t) \cdot \langle u \rangle \, dx. \tag{2.2}$$

From this it is clear that the effect of the fluctuations on the mean flow is contained in $\int R(u,u) : \langle u \rangle \, dx$. When this term is positive, the effect is dissipative and when negative the effect is to increase energy in the mean flow.

Theorem 2.3 (Variance Evolution). *The variance of strong solutions of the NSE evolves according to*

$$\frac{1}{2}V(u(T)) + \int_0^T \nu V(\nabla u(t)) dt = \frac{1}{2}V(u(0)) + \int_0^T \left(\int_\Omega R(u,u) : \langle u \rangle \, dx \right) dt. \tag{2.3}$$

Proof. The energy equality for strong solutions of each realization of the NSE is

$$\frac{1}{2}||u_j(T)||^2 + \int_0^T \nu||\nabla u_j||^2 dt = \frac{1}{2}||u_j(0)||^2 + \int_0^T (f(x,t), u_j) \, dt.$$

Taking the ensemble average of this gives

$$\frac{1}{2} \left\langle ||u_j(T)||^2 \right\rangle + \int_0^T \nu \left\langle ||\nabla u_j||^2 \right\rangle dt = \frac{1}{2} \left\langle ||u_j(0)||^2 \right\rangle + \int_0^T (f(x,t), \langle u_j \rangle) \, dt.$$

Subtract from this the time integral of the equation (2.2). This yields the claimed equation for evolution of variance. ∎

One consequence of the variance evolution equation is a simple proof of the Boussinesq assumption that turbulent fluctuations (defined by ensemble averaging) are dissipative on the mean flow in a mean sense. See [29] for connections to phenomenology. When the means (and thus fluctuations) are defined by long time averaging, a proof of the Boussinesq assumption has been given by Chacon-Rebollo and Lewandowski [5].

Corollary 2.4 (Boussinesq assumption in both $2d$ and $3d$). *Assume* $f(x,t) \in L^{\infty}(0,\infty; L^2(\Omega))$. *For strong solutions of the NSE we have*

$$\lim\inf_{T\to\infty} \frac{1}{T}\int_0^T \left(\int_\Omega R(u,u) : \langle u\rangle \, dx\right) dt = \lim\inf_{T\to\infty} \frac{1}{T}\int_0^T \nu \left\langle ||\nabla u_j'||^2 \right\rangle \geq 0.$$

Proof. For the proof we note that a standard estimate shows that each solution is uniformly bounded $u_j \in L^{\infty}(0,\infty; L^2(\Omega))$. Thus, $V(u) \in L^{\infty}(0,\infty)$. Dividing (2.3) by T we have

$$\frac{1}{2}\frac{1}{T}V(u(T)) + \frac{1}{T}\int_0^T \nu V(\nabla u(t))dt = \frac{1}{2}\frac{1}{T}V(u(0)) + \frac{1}{T}\int_0^T \left(\int_\Omega R(u,u) : \langle u\rangle \, dx\right) dt.$$

As $T \to \infty$ this is

$$\mathcal{O}\left(\frac{1}{T}\right) + \frac{1}{T}\int_0^T \nu \left\langle ||\nabla u_j'||^2 \right\rangle dt = \mathcal{O}\left(\frac{1}{T}\right) + \frac{1}{T}\int_0^T \left(\int_\Omega R(u,u) : \langle u\rangle \, dx\right) dt.$$

The claimed result now follows. $\square$

This shows that on (time) average, the action of the Reynolds stresses / fluctuations in the NSE in both $2d$ and $3d$ (in bounded domains) is

- To dissipate energy in the mean flow $\langle u\rangle$.
- To act as an energy source to the variance evolution equation (2.3) and thus increase variance.

From this analysis, we also see that in a conventional turbulence model the fluctuations should damp both the mean flow and its variance evolution (to approach statistical equilibrium). (In contrast, in a large eddy simulation model, not considered herein, it should on average damp the mean flow but act as a diminished energy source to the model variance equation.)

Remark 2.5. *There are still important open questions concerning the generality of the Boussinesq assumption. In case where means are defined by time averages (see [5]), it is an open question when* $f = f(x,t)$ *and there are questions about whether some version of the result could hold independent of choice of subsequences. When averages are defined by ensemble averaging, [29], the above proof holds when* $f = f(x,t)$ *but not when* $f = f_j(x,t)$. *Extending the above results to weak solutions is also an open problem.*

3. Derivation of the Realization Equation. Consider an ensemble, u_j, p_j, of solutions of the Navier-Stokes equations (NSE) in a regular domain in $\mathbb{R}^d$, $d = (2,3)$:

$$\begin{aligned} &u_{j,t} + u_j \cdot \nabla u_j - \nu \triangle u_j + \nabla p_j = f_j(x,t), \text{ in } \Omega,\ j = 1,...,J, \\ &\nabla \cdot u_j = 0, \text{ and } u_j(x,0) = u_j^0(x), \text{ in } \Omega \text{ and } u_j = 0, \text{ on } \partial\Omega. \end{aligned} \tag{ENSE}$$

If a direct numerical simulation of the NSE were possible, (ENSE) could be solved then averaged to obtain k' for (1.1). Naturally, this is infeasible in many cases. We thus seek stabilized realization equations with the correct ensemble average (1.1) . Define the ensemble mean $\langle u\rangle$**,** fluctuation u_j', its magnitude $|u'|$ and the induced kinetic energy density k' by

$$\langle u\rangle := \frac{1}{J}\sum_{j=1}^{J} u_j, \quad u_j' := u_j - \langle u\rangle\,,$$

$$|u'|^2 := \sum_{j=1}^{J} |u_j'|^2 \text{ and } k'(x,t) = \frac{1}{2}\ |u'|^2(x,t).$$

There are a number of ways to choose the mixing length l including the common choice $l = \triangle x$, the mesh width. In [19], an alternative mixing length

$$l = \text{ \textit{distance a fluctuating eddy travels in one time step}} = |u'|\triangle t,$$

yielded better flow predictions, better stability and $l(x) \to 0$ correctly as $x \to$ walls. Thus, take

$$l = \ |u'|\triangle t.$$

Taking the ensemble average of (ENSE) gives

$$\langle u \rangle_t + \langle u \rangle \cdot \nabla \langle u \rangle - \nu \triangle \langle u \rangle + \nabla \cdot R(u,u) + \nabla \langle p \rangle = \langle f \rangle . \tag{3.1}$$

EV models result from *replacing the Reynolds stress term by the eddy viscosity term.*

Thus, we solve *a feasible variation on (ENSE) which, upon ensemble averaging, yields the correct EV model (1.1) above.* Adding, a yet to be determined, $\nabla \cdot Q_j$ to (ENSE) gives

$$u_{j,t} + u_j \cdot \nabla u_j - \nu \triangle u_j + \nabla \cdot Q_j + \nabla p_j = f_j(x,t). \tag{3.2}$$

Taking the ensemble average of the perturbed equation and rearranging gives

$$\langle u \rangle_t + \langle u \rangle \cdot \nabla \langle u \rangle - \nu \triangle \langle u \rangle + \nabla \cdot \langle Q \rangle - \nabla \cdot R(u,u) + \nabla \langle q \rangle = \langle f(x,t) \rangle . \tag{3.3}$$

Comparing (3.3) and (1.1), we must have (model terms incorporated in the pressure)

$$\begin{aligned} &\langle Q \rangle = \langle u \rangle \langle u \rangle - \langle uu \rangle - \nu_T(l,k') \nabla \langle u \rangle \text{ , or} \\ &Q_j = Term1 - u_j u_j - \nu_T(l,k') \nabla u_j \text{ where } < Term1 >= \ \langle u \rangle \langle u \rangle . \end{aligned}$$

The three natural choices for $Term1$ (all worthy of study) that satisfy $< Term1 > = \langle u \rangle \langle u \rangle$ are $Term1{=}\langle u \rangle \langle u \rangle$, $u_j \langle u \rangle$ and $\langle u \rangle u_j$. These yield

$$\begin{aligned} &Q_j = \langle u \rangle \langle u \rangle - u_j u_j - \nu_T(l,k') \nabla u_j, \\ &Q_j = u_j \langle u \rangle - u_j u_j - \nu_T(l,k') \nabla u_j, \text{ and} \\ &Q_j = \langle u \rangle u_j - u_j u_j - \nu_T(l,k') \nabla u_j \ . \end{aligned}$$

Combinations of these three possibilities also satisfy $< Term1 > = \langle u \rangle \langle u \rangle$. We select the third, Leray inspired, [21], [22], for testing the realization equation

$$u_{j,t} + \langle u \rangle \cdot \nabla u_j - \nabla \cdot ([\nu + \nu_T(l,k')] \nabla u_j) + \nabla p_j = f_j(x,t). \tag{3.4}$$

This is an ensemble-Leray regularization with an eddy viscosity term. Experience with both Leray regularizations (proven robust in computations when the average is smoothing, e.g., [13]) and eddy viscosity models suggests that this realization equation is computationally feasible. The analysis in Section 4 supports this conclusion.

Remark 3.1. *Adding eddy viscosity to all equations, studied in [19], leads to the realization equation*

$$u_{j,t} + u_j \cdot \nabla u_j - \nabla \cdot ([\nu + \nu_T(l,k')] \nabla u_j) + \nabla p_j = f_j(x,t). \tag{3.5}$$

Taking the ensemble average of the (3.5) *gives*

$$\begin{aligned} &\langle u \rangle_t + \langle u \rangle \cdot \nabla \langle u \rangle - \nu \triangle \langle u \rangle + \nabla \langle q \rangle \\ &+ \nabla \cdot R(u,u) - \nabla \cdot (\nu_T(l,k') \nabla \langle u \rangle) = \langle f(x,t) \rangle , \end{aligned}$$

containing both the Reynolds stresses and the EV term. Thus, in (3.5)*, EV is a numerical regularization and not a closure model since it does not replace the Reynolds stresses.*

Analysis. The realization equation (3.4) contains two new effects: the eddy viscosity term and the advection with correlated advecting velocity (i.e., replacing $u_j \cdot \nabla u_j$ by $\langle u \rangle \cdot \nabla u_j$). Before studying their combination we analyze the effect of the latter alone.

Therefore let u_i, u_j be two solutions of

$$u_t + \langle u \rangle \cdot \nabla u - \nu \triangle u + \nabla p = f, \quad \nabla \cdot u = 0. \tag{3.6}$$

subject to the boundary and initial conditions of (ENSE). We prove that the above ensemble Leray regularization suffices to squeeze trajectories together and accelerate convergence to statistical equilibrium.

PROPOSITION 3.2. *Let u_i, u_j be weak solutions to* (3.6)*. If $f_i = f_j$ then*

$$\|u_i(t) - u_j(t)\|^2 \leq e^{-\nu t} \|u_i(0) - u_j(0)\|^2.$$

If $\|f_i - f_j\|_{-1}^2(t) \to 0$ as $t \to \infty$ then $\|u_i - u_j\| \to 0$ as $t \to \infty$.

Proof. $\phi = u_i - u_j$ satisfies $\phi_t + \langle u \rangle \cdot \nabla \phi - \nu \triangle \phi + q = f_i - f_j$, $q = p_i - p_j$. Taking the L^2 inner product with ϕ yields

$$\frac{d}{dt}\frac{1}{2}\|\phi\|^2 + \nu \|\nabla \phi\|^2 \leq (f_i - f_j, \phi) \leq \frac{\nu}{2}\|\nabla \phi\|^2 + \frac{1}{2\nu}\|f_i - f_j\|_{-1}^2.$$

By the Poincaré-Friedrichs inequality and using an integrating factor we obtain:

$$\|\phi(t)\|^2 \leq e^{-\nu t}\|\phi(0)\|^2 + \nu^{-1}\int_0^t e^{-\nu(t-s)}\|f_i - f_j\|_{-1}^2(s)ds.$$

If $f_i - f_j \equiv 0$, the first claim follows immediately. For the second, let $\epsilon > 0$ be given. For $\delta > 0$ let τ be large enough that $\|f_i(t) - f_j(t)\|_{-1}^2 < \delta$ for $t \geq \tau$. Then

$$\|\phi(t)\|^2 \leq e^{-\nu t}\|\phi(0)\|^2 + \nu^{-1}\int_0^\tau e^{\nu(s-t)}\|f_i - f_j\|_{-1}^2 ds + \nu^{-1}\int_\tau^t e^{\nu(s-t)}\delta ds.$$

The first term is $< \epsilon/3$ for t large enough as is the second term. The third term is bounded by $\delta\frac{2}{\nu^2}$, which is also $< \epsilon/3$ for δ small enough. Thus $\|\phi(t)\|^2 \to 0$, as claimed. ◻

4. Methods and Stability.

In this section, we study the first order method (1.4) and give a second order method for the realization equation (1.2) and prove their unconditional, long-time, nonlinear stability. The proof of stability is independent of any special techniques for spacial discretization. Thus the spacial discretization will be suppressed and the methods and analysis given for the continuous space, discrete time context. Extension to discrete space adds only notational complexity.

We use standard notation for Lebesgue and Sobolev spaces and their norms. Let $\|\cdot\|$ and $(\cdot,\cdot)$ be the $L^2(\Omega)$ norm and the inner product, respectively. The $L^p(\Omega)$ norm and the Sobolev $W_p^k(\Omega)$ norm are represented by $\|\cdot\|_{L^p}$ and $\|\cdot\|_{W_p^k}$. $H^k(\Omega)$ is the Sobolev space $W_2^k(\Omega)$, with norm $\|\cdot\|_k$.

4.1. The First Order Method.

Let $t^n := n\Delta t$, $n = 0, 1, 2, ..., N$, and $T := N\Delta t$. Denote $u_j^n = u_j(t^n)$, $j = 1, ..., J$. The first order time accurate method is: *Given u_j^n, find u_j^{n+1}, p_j^{n+1} satisfying*

$$\begin{gathered}\frac{u_j^{n+1} - u_j^n}{\Delta t} + \langle u \rangle^n \cdot \nabla u_j^{n+1} + \nabla p_j^{n+1} \\ -\nu \Delta u_j^{n+1} - \nabla \cdot (2\nu_T(l^n, k'^n)\nabla^s u_j^{n+1}) = f_j^{n+1} \text{ in } \Omega, \\ \text{where } \nu_T(l^n, k'^n) = \mu |u'^n| l^n \text{ and } l^n = |u'^n|\Delta t, \\ \nabla \cdot u_j^{n+1} = 0, \text{ and } u_j^0(x) = u_j^0 \text{ in } \Omega, \; u_j^{n+1} = 0, \text{ on } \partial\Omega\end{gathered} \tag{4.1}$$

After spacial discretization, every time step of (4.1) requires the solution of a block linear system like (1.3) with shared coefficient matrix.

We prove unconditional stability of (4.1).

THEOREM 4.1 (Stability of the first order method). *The first order method* (4.1) *is unconditionally stable*

$$||u_j^N||^2 + \sum_{n=0}^{N-1}\left(||u_j^{n+1}-u_j^n||^2 + \triangle t\int_\Omega [\nu+\nu_T(l^n,k'^n)]|\nabla u_j^{n+1}|^2 dx\right) \tag{4.2}$$
$$\leq ||u_j^0||^2 + \frac{\triangle t}{\nu}\sum_{n=0}^{N-1}\|f_j^{n+1}\|_{-1}^2.$$

The ensemble average is also similarly stable:

$$||\left\langle u\right\rangle^N||^2 + \sum_{n=0}^{N-1}\left(||\left\langle u\right\rangle^{n+1}-\left\langle u\right\rangle^n||^2 + \triangle t\int_\Omega [\nu+\nu_T(l^n,k'^n)]|\nabla\left\langle u\right\rangle^{n+1}|^2 dx\right)$$
$$\leq ||\left\langle u\right\rangle^0||^2 + \frac{\triangle t}{\nu}\sum_{n=0}^{N-1}\|\left\langle f\right\rangle^{n+1}\|_{-1}^2. \tag{4.3}$$

Proof. We take the L^2 inner product of the first equation of (4.1) with u_j^{n+1}, the second equation with p_j^{n+1}, add and multiply by $2\triangle t$. Using skew symmetry $\int_\Omega \left\langle u\right\rangle^n\cdot\nabla u_j^{n+1}.u_j^{n+1}\,dx = 0$, the polarization identity for (u_j^n, u_j^{n+1}) in the time difference term and integrating by parts the two viscosity terms gives

$$||u_j^{n+1}||^2 - ||u_j^n||^2 + ||u_j^{n+1}-u_j^n||^2 + 2\triangle t\int_\Omega [\nu+\nu_T(l^n,k'^n)]|\nabla u_j^{n+1}|^2 dx \tag{4.4}$$
$$= 2\triangle t\left(f_j^{n+1}, u_j^{n+1}\right).$$

Applying Young's inequality to the right hand side

$$||u_j^{n+1}||^2 - ||u_j^n||^2 + ||u_j^{n+1}-u_j^n||^2$$
$$+\triangle t\int_\Omega [\nu+2\nu_T(l^n,k'^n)]|\nabla u_j^{n+1}|^2 dx \leq \frac{\triangle t}{\nu}\|f_j^{n+1}\|_{-1}^2.$$

Long-time stability of the realization thus follows. For (4.3), ensemble average (4.1) (giving (1.1)), then, repeat the proof. ▯

The two energy inequalities (4.2), (4.3) are key steps for establishing convergence to statistical equilibrium.

PROPOSITION 4.2 (Variance Evolution of the First Order Method). *Suppose in* (4.1) $f_j \equiv f$. *The variance of solutions to* (4.1) *evolves according to*

$$V(u^N) + \sum_{n=0}^{N-1}\Big\{V(u^{n+1}-u^n) \tag{4.5}$$
$$+\Delta t\int_\Omega [\nu+\nu_T(l^n,k'^n)]\left\langle|\nabla u_j'^{n+1}|^2\right\rangle dx\Big\} = V(u^0).$$

Proof. Take the ensemble average of (4.4) and of the analogous step in the energy estimate for $\| < u >^N \|$ then subtract to obtain variance evolution. Note that since $f_j \equiv f$, the RHS cancel:

$$\left\langle 2\Delta t(f^{n+1}, u_j^{n+1})\right\rangle - 2\Delta t(f^{n+1}, \left\langle u_j^{n+1}\right\rangle) \equiv 0.$$

We then have

$$
\begin{gathered}
V(u^{n+1}) - V(u^n) + V(u^{n+1} - u^n) \\
+\Delta t \int_\Omega [\nu + \nu_T(l^n, k'^n)] \left\langle |\nabla u_j'^{n+1}|^2 \right\rangle dx = 0.
\end{gathered}
$$

Summing from $n = 0$ to $N - 1$ gives the result. □

This proposition has several important consequences. In particular, we conclude that when $f_j \equiv f \in L^\infty(0, \infty; L^2(\Omega))$, $V(u^N) \to 0$ as $t^N \to \infty$.

Proposition 4.3. *In* (4.1) *let* $f_j \equiv f \in L^\infty(0, \infty; L^2(\Omega))$. *Then, as* $t^N \to \infty$

$$
\begin{gathered}
V(u^{N+1} - u^N) \to 0, \\
V(\nabla u^N) \to 0, \\
\int_\Omega \nu_T(l^N, k'^N) \left\langle |\nabla u_j'^{N+1}|^2 \right\rangle dx \to 0.
\end{gathered}
$$

Proof. Each term in (4.5) is nonnegative and the RHS is independent of N. Letting $N \to \infty$ we conclude that the infinite series (with nonnegative terms) below converges

$$
\sum_{n=0}^{\infty} \left\{ V(u^{n+1} - u^n) + \Delta t \nu V(\nabla u^{n+1}) + \Delta t \int_\Omega \nu_T(l^n, k'^n) \left\langle |\nabla u_j'^{n+1}|^2 \right\rangle dx \right\} < \infty.
$$

Thus, the N^{th} term must $\to 0$ as $N \to \infty$ and the proposition follows. □

Remark 4.4. *For the proofs to hold in the discrete space case requires the two viscosity terms to yield SPD matrices (i.e., be dissipative under discretization) and the discrete nonlinear term to be skew symmetric (i.e., conservative) or nonnegative (i.e., add numerical dissipation via some upwinding).*

4.2. The Second Order Method. The second order time accurate method for (1.2) is a combination of $BDF2$ and an interpretation of $AB2$ for the nonlinear term. The second order accurate method is as follows: *Given* u_j^{n-1}, u_j^n, *find* u_j^{n+1}, p_j^{n+1} *satisfying*

$$
\begin{gathered}
\frac{3u_j^{n+1} - 4u_j^n + u_j^{n-1}}{2\Delta t} + \Big(2\left\langle u\right\rangle^n - \left\langle u\right\rangle^{n-1}\Big) \cdot \nabla u_j^{n+1} + \nabla p_j^{n+1} \\
-\nu \triangle u_j^{n+1} - \nabla \cdot \left(\tilde{\nu}_T(l^n, k'^n) \nabla^s u_j^{n+1}\right) = f_j^{n+1} \text{ in } \Omega, \\
\text{where } \tilde{\nu}_T(l^n, k'^n) = \mu |2u'^n - u'^{n-1}| l^n \text{ and } l^n = |2u'^n - u'^{n-1}| \Delta t, \\
\nabla \cdot u_j^{n+1} = 0, \text{ and } u_j^0(x) = u_j^0 \text{ in } \Omega, u_j^{n+1} = 0, \text{ on } \partial\Omega.
\end{gathered}
\tag{4.6}
$$

This is a 3 level/2 step method. Thus an approximation to u_j^1, p_j^1 must be computed by some other method, such as the first order method (4.1) above. Like the first order method, it is unconditionally stable.

Theorem 4.5 (Stability of the second order method). *The second order method (4.6) is unconditionally, long-time, nonlinear stable: For any* $N > 1$,

$$
\begin{aligned}
&\frac{1}{4}\|u_j^N\|^2 + \frac{1}{4}\|2u_j^N - u_j^{N-1}\|^2 + \sum_{n=1}^{N-1} \frac{1}{4}\|u_j^{n+1} - 2u_j^n + u_j^{n-1}\|^2 \\
&+\Delta t \sum_{n=1}^{N-1} \int_\Omega \tilde{\nu}_T(l^n, k'^n) |\nabla u_j^{n+1}|^2 dx + \frac{\Delta t}{2} \sum_{n=1}^{N-1} \nu \|\nabla u_j^{n+1}\|^2 \\
&\leq \sum_{n=1}^{N-1} \frac{\Delta t}{2\nu} \|f_j^{n+1}\|_{-1}^2 + \frac{1}{4}\|u_j^1\|^2 + \frac{1}{4}\|2u_j^1 - u_j^0\|^2 \ .
\end{aligned}
$$

Proof. Take the L^2 inner product of (4.6) with u_j^{n+1}, p_j^{n+1} and add. Using skew-symmetry of the nonlinear term, integrating by parts the two viscous terms, canceling the pressure and incompressibility terms and multiplying through by Δt yields:

$$\begin{aligned} &\frac{1}{4}\left(\|u_j^{n+1}\|^2 + \|2u_j^{n+1} - u_j^n\|^2\right) - \frac{1}{4}\left(\|u_j^n\|^2 + \|2u_j^n - u_j^{n-1}\|^2\right) \\ &+\frac{1}{4}\|u_j^{n+1} - 2u_j^n + u_j^{n-1}\|^2 + \int_\Omega \Delta t\left(\nu + \tilde{\nu}_T(l^n, k'^n)\right)|\nabla u_j^{n+1}|^2 dx \\ &= \Delta t\left(f_j^{n+1}, u_j^{n+1}\right) \ . \end{aligned} \tag{4.7}$$

Applying Young's inequality to the right hand side gives

$$\begin{aligned} &\frac{1}{4}\left(\|u_j^{n+1}\|^2 + \|2u_j^{n+1} - u_j^n\|^2\right) - \frac{1}{4}\left(\|u_j^n\|^2 + \|2u_j^n - u_j^{n-1}\|^2\right) \\ &+\frac{1}{4}\|u_j^{n+1} - 2u_j^n + u_j^{n-1}\|^2 + \int_\Omega \Delta t\left(\nu + \tilde{\nu}_T(l^n, k'^n)\right)|\nabla u_j^{n+1}|^2 dx \\ &\leq \frac{\nu\Delta t}{2}\|\nabla u_j^{n+1}\|^2 + \frac{\Delta t}{2\nu}\|f_j^{n+1}\|_{-1}^2 \ . \end{aligned}$$

Combining like terms yields

$$\begin{aligned} &\frac{1}{4}\left(\|u_j^{n+1}\|^2 + \|2u_j^{n+1} - u_j^n\|^2\right) - \frac{1}{4}\left(\|u_j^n\|^2 + \|2u_j^n - u_j^{n-1}\|^2\right) \\ &+\frac{1}{4}\|u_j^{n+1} - 2u_j^n + u_j^{n-1}\|^2 + \int_\Omega \Delta t\left(\frac{\nu}{2} + \tilde{\nu}_T(l^n, k'^n)\right)|\nabla u_j^{n+1}|^2 dx \leq \frac{\Delta t}{2\nu}\|f_j^{n+1}\|_{-1}^2 \ . \end{aligned} \tag{4.8}$$

Summing up (4.8) from $n = 1$ to $N - 1$ completes the proof. □

The second order method also produces approximations that approach statistical equilibrium (by Variance $\to 0$) in the same sense as for the first order method.

Proposition 4.6 (Variance Evolution of Second Order Method). *Suppose in* (4.6) $f_j \equiv f$. *The variance of solutions to* (4.6) *satisfies*

$$\begin{aligned} &V(u^N) + V(2u^N - u^{N-1}) + \sum_{n=1}^{N-1}\Big\{V(u^{n+1} - 2u^n + u^{n-1}) \\ &+4\Delta t\int_\Omega \left(\nu + \tilde{\nu}_T(l^n, k'^n)\right)\left\langle|\nabla u_j'^{n+1}|^2\right\rangle dx\Big\} = V(u^1) + V(2u^1 - u^0). \end{aligned} \tag{4.9}$$

Proof. The ensemble average of (4.7) and of the analogous step in the energy estimate for $\| \langle u\rangle^N \|$ yields

$$\begin{aligned} &V(u^{n+1}) + V(2u^{n+1} - u^n) - V(u^n) - V(2u^n - u^{n-1}) \\ &+V(u^{n+1} - 2u^n - u^{n-1}) + 4\Delta t\int_\Omega \left(\nu + \tilde{\nu}_T(l^n, k'^n)\right)\left\langle|\nabla u_j'^{n+1}|^2\right\rangle dx = 0. \end{aligned}$$

Summing from $n = 1$ to $N - 1$ gives the result. □

Proposition 4.7. *In* (4.6) *let* $f_j \equiv f \in L^\infty(0,\infty; L^2(\Omega))$. *Then, as* $t^N \to \infty$

$$\begin{aligned} V(u^{N+1} - 2u^N + u^{N-1}) &\to 0, \\ V(\nabla u^N) &\to 0, \\ \int_\Omega \tilde{\nu}_T^n \left\langle|\nabla u_j'^{N+1}|^2\right\rangle dx &\to 0. \end{aligned}$$

Proof. Note that each term in (4.9) is nonnegative and the RHS is independent of N. Letting $N \to \infty$ we conclude that the infinite series (with nonnegative terms) below converges

$$\sum_{n=1}^{\infty} \left\{ V(u^{n+1} - 2u^n + u^{n-1}) + \Delta t \nu V(\nabla u^{n+1}) + \Delta t \int_{\Omega} \tilde{\nu}_T(l^n, k'^n) \left\langle |\nabla u_j'^n|^2 \right\rangle dx \right\} < \infty.$$

Thus, the N^{th} term must $\to 0$ as $N \to \infty$ and the proposition follows. ◻

5. Numerical Experiments.

5.1. Comparing two realization equations. In this section, we investigate the difference between retaining and not retaining the fluctuating term $u_j' \cdot \nabla u_j$ (equivalently, retaining in the ensemble averaged equation both the Reynolds stresses and the eddy viscosity or just the eddy viscosity). While these first tests are $2d^2$, they reveal differences between ensemble numerical regularizations (retaining $u_j' \cdot \nabla u_j$) and turbulence models (not retaining $u_j' \cdot \nabla u_j$).

Test Problem: flow between offset circles. Pick

$$\Omega = \{(x, y) : x^2 + y^2 \le r_1^2 \text{ and } (x - c_1)^2 + (y - c_2)^2 \ge r_2^2\},$$
$$r_1 = 1, r_2 = 0.1, c = (c_1, c_2) = (\frac{1}{2}, 0),$$
$$f(x, y, t) = (-4y(1 - x^2 - y^2), 4x(1 - x^2 - y^2))^T,$$

with no-slip boundary conditions on both circles. The flow, driven by a counterclockwise force (with $f \equiv 0$ at the outer circle), rotates about $(0, 0)$ and interacts with the immersed circle. This induces a von Kármán vortex street which interacts with the near wall streaks common in turbulent flow and a central ("polar") vortex. All three effects interact in a pulsating fashion. We discretize in space using the usual finite element method with Taylor-Hood elements, [30]. These choices satisfy the requirements for the stability theorems to apply. The tests were performed using FreeFEM++, [16]. The mesh has $n = 40$ mesh points around the outer circle and $m = 10$ mesh points around the immersed circle, and extended to Ω as a Delaunay mesh.

Generation of the initial conditions. Initial conditions $u_j^0, j = 1, 2,$ and u_0^0, are generated by solving the steady Stokes problem with body forces

$$f(x, y, 0) + \epsilon(sin(3\pi x)sin(3\pi y), cos(3\pi x)cos(3\pi y))^T,$$

taking $\epsilon = 10^{-3}, -10^{-3}$ and 0. These initial conditions give u_1, u_2, $u_{ave} = (u_1 + u_2)/2$ and u_0 (initial condition u_0^0 -'no perturbation'). Thus we perturb the small scales rather than generate bred vectors herein.

Comparing realization equations (3.4) **vs** (3.5)

We compare the stability of the two choices and test the relative size (residual) of the extra term $u_j' \cdot \nabla u_j$. For stability, we choose a large time step and compute the kinetic energy vs time and enstrophy vs time t over $0 \le t \le 10$

$$\text{Energy} = \frac{1}{2}\|u\|^2, \quad \text{Enstrophy} = \frac{1}{2}\nu\|\nabla \times u\|^2.$$

The plots are given in Figures 5.1 and 5.2 below.

Comparing the cases in Figure 5.1 (energy) and 5.2 (enstrophy) we see that EV as a turbulence model (the lower figure) produces fewer transient effects than adding EV as a numerical regularization (the top figure). This is consistent with considering the methods studied as conventional turbulence models.

[2] Bounded domains are not covered by the Batchelor-Leith-Kraichnan inverse cascade. On bounded 2d domains under no-slip boundary conditions fluctuations have a dissipative effect on the mean flow (consistent with an eddy viscosity model), Section 2 above, [28], [29], see also [31]. Thus, this test is sensible.

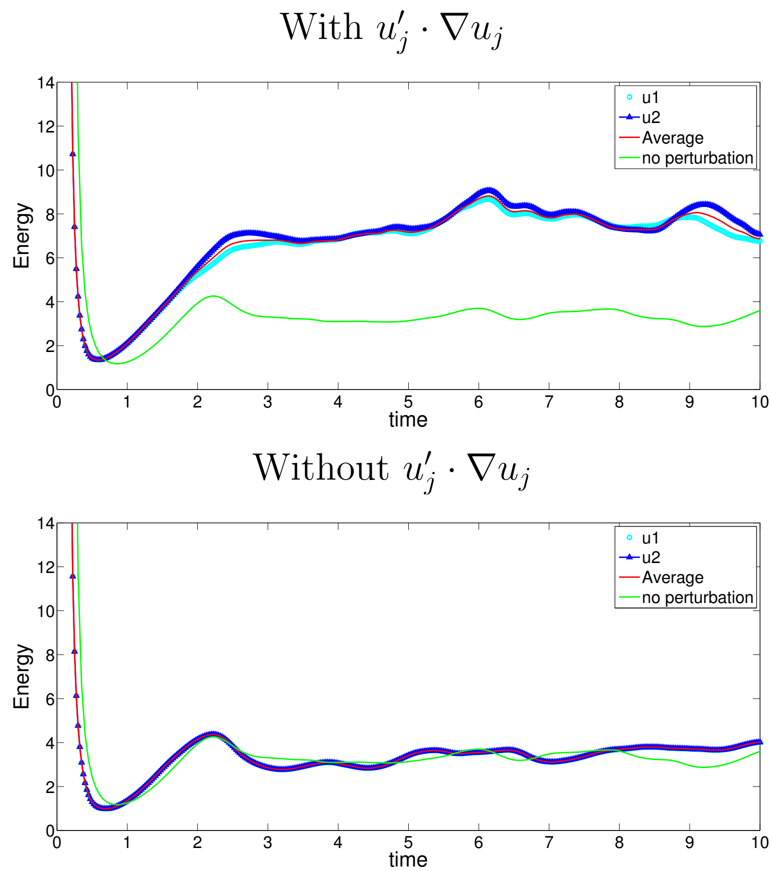

FIG. 5.1. *Energy,* $\nu = 1/800$, $\Delta t = 0.025$.

The realization equation (1.2) (with nonlinear term $\langle u \rangle \cdot \nabla u_j$) is consistent with the desired statistical turbulence model (1.1). However, as $u_j \cdot \nabla u_j =< u > \cdot \nabla u_j + u_j' \cdot \nabla u_j$, it is not a consistent approximation to the NSE as it omits $u_j' \cdot \nabla u_j$. We test the magnitude of $u_j' \cdot \nabla u_j$. Next, the test investigates the relative size of the extra term $u_j' \cdot \nabla u_j$. We measure the relative significance of both terms by computing over $0 \leq t \leq 10$

$$Q_1 = \left\langle || \langle u \rangle^n \cdot \nabla u_j^{n+1} ||^2 \right\rangle, \quad Q_2 = \left\langle ||(u_j^n - \langle u \rangle^n) \cdot \nabla u_j^n ||^2 \right\rangle,$$
$$Q_3 = \frac{\left\langle ||(u_j^n - \langle u \rangle^n) \cdot \nabla u_j^n ||^2 \right\rangle}{\left\langle || \langle u \rangle^n \cdot \nabla u_j^{n+1} ||^2 \right\rangle}.$$

Figure 5.3 plots the three vs time.

Figure 5.3 shows that the relative difference between the realization equations (3.4) and (3.5) is a term that is smaller than 10^{-10}. Nevertheless, the impact of the extra term on the kinetic energy is $\mathcal{O}(1)$, Figure 5.1. Excluding $u' \cdot \nabla u$, the energy and enstrophy closely track the unperturbed flow (bottom Figure 5.1, 5.2).

We concluded from this first test that the term is small in magnitude but non-negligible as its effects on the transient evolution of the flow.

5.2. Interrogation of Convergence to Statistical Equilibrium. One goal of a conventional turbulence model is for its time evolution to very quickly converge to the statistical equilibrium of the flow. We test this convergence by computing the averaged, effective Lyapunov exponents (introduced by [3]) of the first order method. Negative exponents imply exponential convergence to equilibrium.

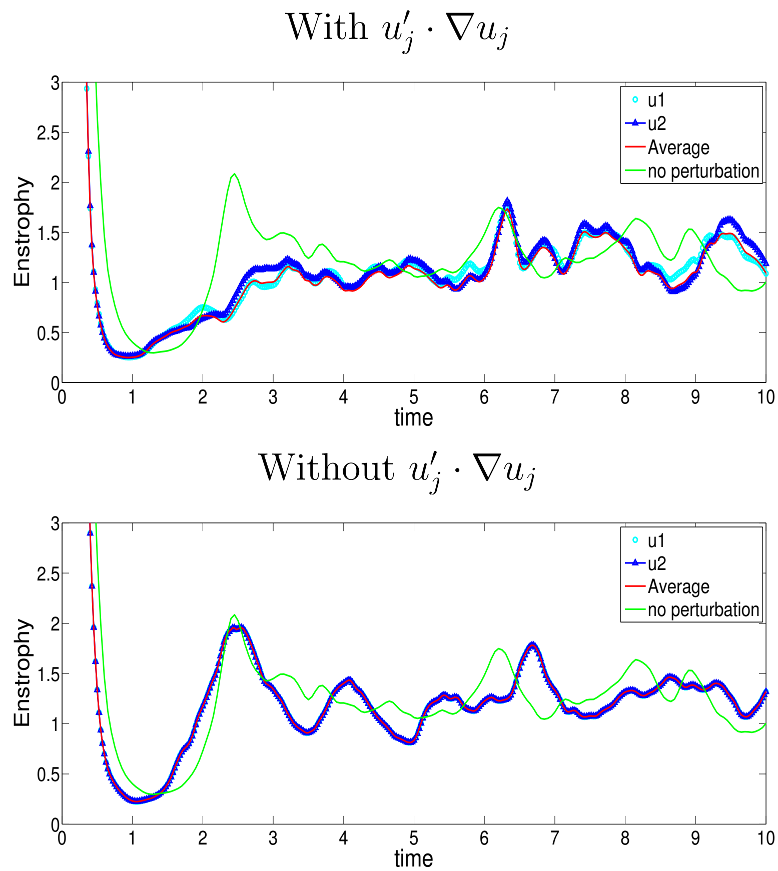

FIG. 5.2. *Enstrophy,* $\nu = 1/800$*,* $\Delta t = 0.025$*.*

Following [3], we define the **relative energy fluctuation** $r(t)$ by

$$r(t) := \frac{\|u_1 - u_2\|^2}{\|u_1\|\|u_2\|}(t),$$

and the **averaged, effective Lyapunov exponent** $\gamma_T(t)$ over $0 \le t \le T$ by

$$\gamma_T(t) := \frac{1}{2T} log\left(\frac{r(t+T)}{r(t)}\right).$$

Here T is chosen to be the simulation time.

From figure 5.4 we see that around $t = 2$ the Lyapunov exponent became negative (and stay negative thereafter), indicating squeezing of the trajectories, as predicted by the theory.

If the solution converges to steady state (physical equilibrium) then as $\frac{d}{dt}\langle u \rangle = 0$ it must be a solution of the steady NSE. At $t^{n+1} = 10$, we compute $\| \langle u \rangle^{n+1} - \langle u \rangle^{n} \| = 0.24256$. This shows the model is not at steady state. On the other hand, $V(\nabla u^{n+1}) = 2.72848^{-12}$ at $t^{n+1} = 10$, which is a clear evidence that the model has reached its statistical equilibrium. This is consistent with the fact the statistically averaged mean flow can be unsteady, clearly illustrated in Figure 5.12, page 102 in [8].

In order to visualize the evolution of the flow we plot vorticity contours of $\langle u \rangle^n$ in Figure 5.5. To resolve the vortices around the inner circle, we compute on a finer mesh (still relatively coarse) with 150 mesh points on the outer circle and with 75 mesh points on the inner circle. Two apparent oppositely-rotating vortices shedding from the inner circle are

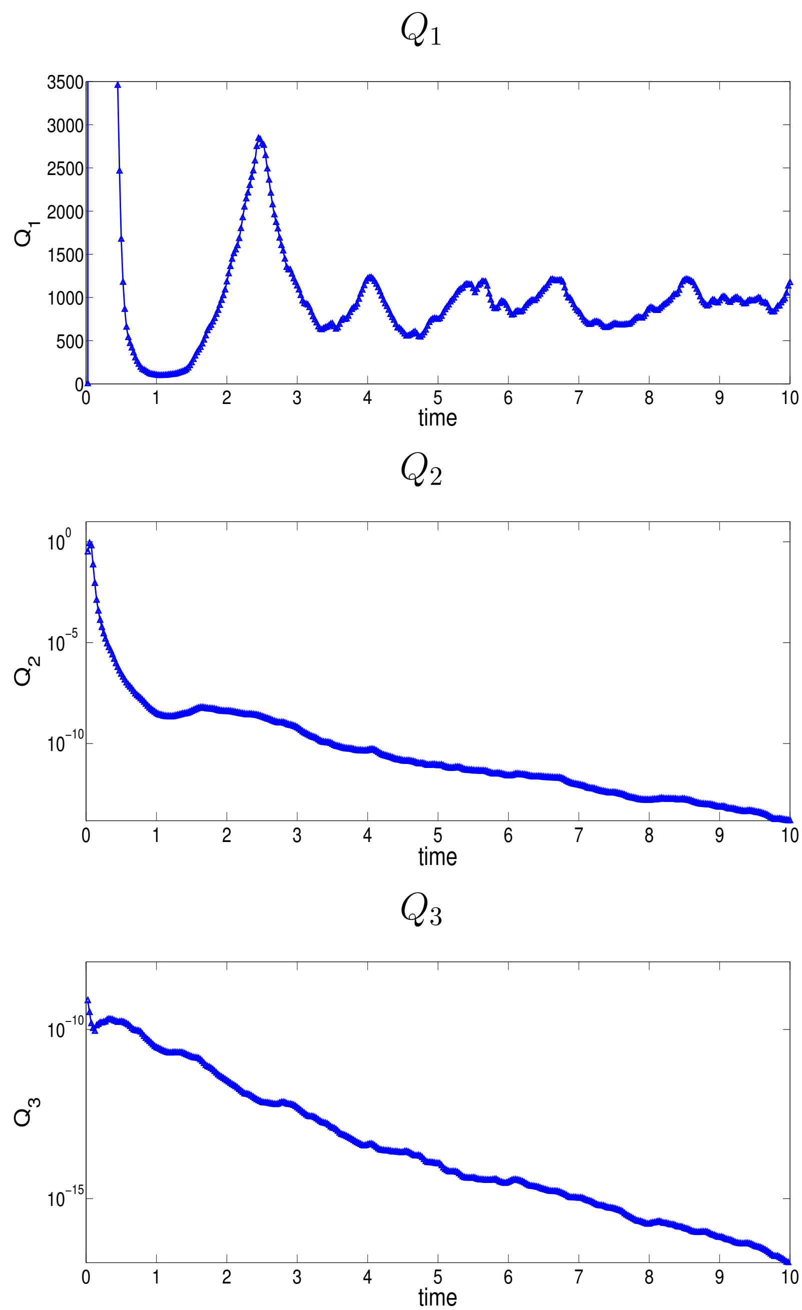

FIG. 5.3. $\nu = 1/800$, $\Delta t = 0.025$, *without* $u'_j \cdot \nabla u_j$

observed at very early time (clear at $t = 1$, Figure 5.5). An animation of the flow also shows many interesting features. The two oppositely-rotating vortices are shed and detach from the inner circle periodically. On the other hand, the near wall streaks appear and disappear in a pulsating fashion and also a central ("polar") vortex appear and disappear. The eddies are shed by the inner circle sometimes break up into streaks and sometimes are captured by a large central vortex.

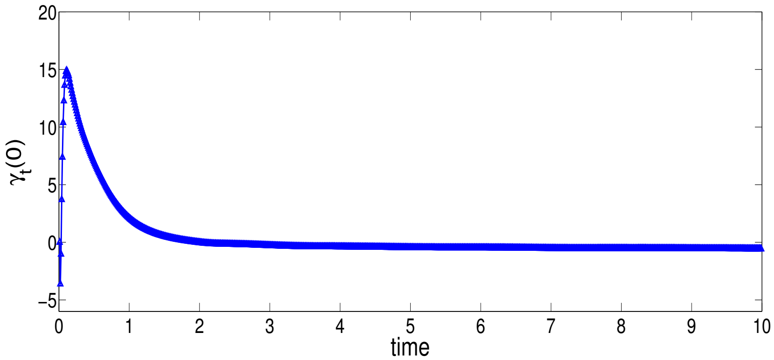

FIG. 5.4. *Averaged, effective Lyapunov exponent,* $\nu = 1/800$, $\Delta t = 0.01$.

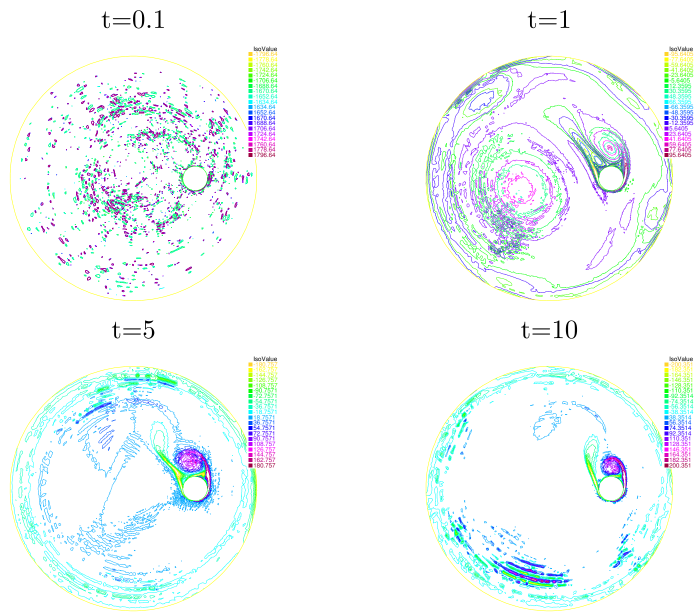

FIG. 5.5. *Vorticity,* $\nu = 1/800$, $\triangle t = 0.01$.

6. Conclusions and Open Questions. In fluid dynamics it is uncommon for numerical tests to be unequivocal and not unknown for unequivocal tests to be incorrectly interpreted. With this warning in mind, the initial tests suggest that the method (1.1) functions as a very effective conventional turbulence model. Simply adding an EV term to each NSE realization means including the $u_j' \cdot \nabla u_j$ term, [19]. In this case, EV functions as a numerical regularization. The theory and the (simple) tests herein show (Figures 5.1, 5.2, 5.4) that the solution remains much closer to the unperturbed solution and converges to a time averaged statistical equilibrium. (Compare the Lyapunov exponents of the model (1.1) in Figure 5.4 herein to those of the regularization, Figure 8 in [17].) Ensemble simulations with different realization equations provide very effective numerical regularizations and conventional turbulence models.

There are applications such as uncertainty quantification and sensitivity analysis in which calculation of an ensemble of solutions is an essential step. With these applications, developing turbulence models from the calculated ensemble is useful. Further, computing the ensemble at reduced cost based on block methods is promising as well. The methods in this report, as their next step, should be tested in more complex turbulent flow benchmark problems.

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