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A TRANSFER THEORY ANALYSIS OF APPROXIMATE DECONVOLUTION MODELS OF TURBULENCE

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Abstract. This study considers Pao's transfer theory of turbulence for the family of Approximate Deconvolution Models (ADMs). By taking a different representation of the persistent input of energy into the large scales of the turbulent flow, the Pao theory simplifies somewhat. Analysis of the resulting model is given and it is verified that (after the simplification as was known before it) it is consistent with the important statistics of homogeneous isotropic turbulence. The ADMs have an enhanced energy dissipation and a modification to the kinetic energy which affect the truncation of scales by reducing the models microscale from the Kolmogorov microscale. The energy dissipation can be even more enhanced by the time relaxation and the effects of this term are presented as well.

Key words. energy transfer theory, shell model, turbulence, approximate deconvolution.

1. Introduction

Turbulent flows consist of complex, interacting three dimensional eddies of various sizes. In 1941 Kolmogorov gave a remarkable, universal description of the eddies in turbulent flow by combining a judicious mix of physical insight, conjecture, mathematical and dimensional analysis. In his description, the largest eddies are deterministic in nature. Those below a critical size are dominated by viscous forces, and die very quickly due to these forces. This critical length, the Kolmogorov microscale, is $\eta = O(Re^{-3/4})$ in $3d$, so the persistent eddies in a $3d$ flow requires taking $\Delta x = \Delta y = \Delta z = O(Re^{-3/4})$ giving $O(Re^{+9/4})$ mesh points in space per time step. Therefore, direct numerical simulation of turbulent flows (down to the Kolmogorov microscale) is often not computationally economical or even feasible. On the other hand, the largest structures in the flow (containing most of the flow's energy) are responsible for much of the mixing and most of the flow's momentum transport. Thus, various turbulence models are used for simulations seeking to predict a flow's large structures.

One of the mysteries of turbulence is how energy is transferred between scales and how nonlinearity achieves a balance between the input of energy at large scales and its dissipation on exceedingly small scales. In the study of energy transfer among scales, the energy at time t and in scales parameterized by wave-number k, is denoted $E(k,t)$. Energy transfer theories explore this through simplified partial differential equations for $E(k,t)$. Shell models explore the energy transfer among scales by further discretizing the variable k through simplified systems of ordinary differential equations for the energy in a wave-number shell, typically denoted $E_n(t)$ or $u_n(t)$. Transfer theories and shell models have a common aim of understanding a critical feature of turbulent flow and have attracted the attention of many researchers on turbulence so there are a large number of different such models of increasing complexity. Perhaps surprisingly, of these only the simplest Energy Transfer Model of Pao [25] gives unequivocally correct (to the extent that

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the phenomena is understood) predictions of the time averaged statistics and energy spectrum of homogeneous isotropic turbulence. Understanding the mystery of energy transfer through nonlinearity becomes of critical importance in predictions of turbulent flows because one fundamental role of turbulence models is to add $O(1)$ terms which exactly emulate the effects of this not well understood process on scales much larger than the process itself occurs. For example, in 1960 J. Smagorinsky wrote:

> *"In setting up a finite difference grid or a finite wave number space, a turbulent threshold is in effect defined and the question is: How do the equations know how to communicate with the molecular dissipation range? One of course finds empirically that, without any provision for dissipation, the cascade of energy to the higher wave numbers ultimately increases the energy of the smallest wave resolvable by the grid. This energy has no place further to go, and ultimately the calculation departs from nature sufficiently to give intolerable truncation error."* ——— *J. Smagorinsky, 1960*

One promising approach to the simulation of turbulent flows is called *Large Eddy Simulation* or *LES*. Approximate deconvolution models in LES have great promise because they are systematic, have high accuracy and a firm theoretical foundation in some critical respects. The goal of this report is to apply the Pao energy transfer theory to these approximate deconvolution models (ADMs) to gain further insight into their predictions of important turbulent statistics. We derive the energy transfer model associated with ADMs. Interestingly, through a change of variable, the wave-number closure that arises in ADMs becomes exactly the same as the one occurring for the NSE. Thus the Pao closure can be used exactly for the ADM without modification or extra tuning parameters. We thus study the predictions of the Pao transfer theory for ADMs and compare them both theoretically and computationally to those of the NSE. Interestingly, the computational study herein involves wave-number discretization of $E(k,t)$ on wave-number shells (following an equi-partition of energy) and thus results in an apparently new Pao shell model for turbulence.

1.1. The LES Models Considered. In LES the evolution of local, spatial averages over length scales $l \geq \delta$ are sought where δ is user selected. The selection of this averaging radius δ is determined typically by computational resources (δ must be related to the finest computationally feasible mesh), turnaround time needed for the calculation, and estimates of the scales of the persistent eddies needed to be resolved for an accurate simulation. On the face of it, LES seems feasible since the large eddies are believed to be deterministic. The small eddies (accepting Kolmogorov's description) have a universal structure so, in principle, their mean effects on the large eddies should be model-able. The crudest estimate of cost is

$$\Delta x = \Delta y \ = \Delta z = O(\delta), \tag{1}$$

with thus $O(\delta^{-3})$ storage required in space per time step. On the other hand, it is entirely possible that the computational mesh must be smaller than $O(\delta)$ to predict the $O(\delta)$ structures correctly. It is also entirely possible that, since LES models are themselves inexact and uncertain, solutions to an LES model contain persistent energetic structures smaller than $O(\delta)$. Thus, a good LES model will (i) truncate scales so that $microscale = O(\delta)$, consistent with (1), (ii) predict the correct time averaged statistics over scales $l \geq \delta$ (so that computational resolution is free to capture non-universal, non-isotropic, non-fully developed features) and

(iii) be a high accuracy approximation to the NSE over the large scales and capture transitional and other non-fully developed flow behavior.

To introduce the LES models we consider herein, consider first the Navier-Stokes equations in a periodic box $\Omega = (0, L)^3$ in $\mathbb{R}^3$:

$$u_t + u \cdot \nabla u - \nu \triangle u + \nabla p = f \quad \text{and } \nabla \cdot u = 0\,, \tag{2}$$

subject to periodic (with zero mean) conditions, for $j = 1, 2, 3$,

$$u(x + Le_j, t) = u(x, t) \text{ and } \int_\Omega \phi \, dx = 0 \text{ for } \phi = u,\, u_0,\, f,\, p. \tag{3}$$

In deriving equations for velocity averages (denoted $\overline{u}$), many averaging operators are used; herein we choose a differential filter, [12]. Given $\phi(x) \in L^2(\Omega)$, $\overline{\phi}(x)$ is the unique $L-$periodic solution in the Sobolev space $H_1(\Omega)$ of

$$A\overline{\phi} := -\delta^2 \triangle \overline{\phi} + \overline{\phi} = \phi\,, \text{ in } \Omega.$$

Averaging the NSE (meaning: applying A^{-1} to (2)) and noting that $\overline{u \cdot \nabla u} = \nabla \cdot (\overline{uu})$ gives the exact space filtered NSE for $\overline{u}$

$$\overline{u}_t + \nabla \cdot (\overline{uu}) - \nu \triangle \overline{u} + \nabla \overline{p} = \overline{f}\ , \text{ and } \nabla \cdot \overline{u} = 0.$$

This is not closed since $\overline{u\,u} \neq \overline{u}\ \overline{u}$. Approximate deconvolution models are among the most accurate of turbulence models, [1], [2], [30], [9], [18] (see [28], [14], [5] for other models). The van Cittert deconvolution operator (constructed in Section 2 and denoted D_N) was studied by van Cittert in 1931 and its use in LES pioneered by Stolz and Adams [1], [30]. It is an approximate or asymptotic filter inverse satisfying $\phi = D_N(\overline{\phi}) + O(\delta^{2N+2})$ for smooth ϕ. Since $D_N\overline{u}$ approximates u to accuracy $O(\delta^{2N+2})$ in the smooth flow regions it is justified to consider the closure approximation:

$$\overline{uu} \simeq \overline{D_N\overline{u} D_N\overline{u}} + O(\delta^{2N+2}). \tag{4}$$

The resulting models, whose solutions approximate the true flow averages, $w \approx \overline{u}, q \approx \overline{p}$, were introduced by Adams and Stolz [1], [2], [30], and are given by

$$\begin{gathered} w_t + \nabla \cdot (\overline{D_N w\ D_N w}) - \nu \triangle w + \nabla q + \chi\,(w - D_N\overline{w}) = \overline{f}, \\ \nabla \cdot w = 0,\ N = 0, 1, 2, \ldots. \end{gathered} \tag{5}$$

The time relaxation term $\chi\,(w - D_N\overline{w})$ is included in numerical simulations of (5) to damp strongly the temporal growth of the fluctuating component of $w(x, t)$ driven by noise, numerical errors, inexact boundary conditions and so on. It can be used as a numerical regularization in any model and is studied in [2, 19, 27], as well.

In [20] a descriptive turbulence phenomenology was used to study how well (5) predicts universal features of turbulence. Herein we apply a quantitative phenomenology based upon Pao's energy transfer theory to the ADM (5). In doing so, we also develop a new shell theory of turbulence based on the Pao transfer theory which predicts turbulent statistics correctly.

1.2. Summary of results. Beginning with the Pao transfer theory closure, we derive a Pao ADM energy transfer model in Section 3. This energy transfer model gives an approximation for the energy in $D_N w$, which is an approximation to the (energy in the) unfiltered velocity u. We prove in Proposition 4.1 that the Pao-ADM transfer model has a unique solution which has exponential decay for large wavenumbers. For the Pao-ADM, we show in Section 4.1 that the energy dissipation rate (denoted ε_{ADM} and ε_{NSE} respectively) of the underlying flow is correctly estimated

as required for statistical equilibrium: $\varepsilon_{ADM} = O(\varepsilon_{NSE})$. The ADM microscale, where the dissipation range begins, is estimated in Section 4.1 to be

$$\begin{aligned}
\eta_{ADM} &= \eta_{NSE} \doteq Re^{-3/4}L, \text{ when } \delta \leq O(\eta_{NSE}) \text{ and } \chi = 0,\\
\eta_{ADM} &\doteq Re^{-3/10}\delta^{3/5}L, \text{ when } \delta >> O(\eta_{NSE}) \text{ and } \chi = 0,\\
\eta_{ADM} &\doteq \delta, \text{ with } \chi = O(\delta^{-2/3}).
\end{aligned}$$

We also show that $E(k,t)$ converges as $t \to \infty$ to a time averaged spectrum (in Corollary 4.2) which exhibits an inertial range behavior and a dissipation range behavior (see equation (4.2)):

$$E(k) = \frac{1}{2}U^2 k^{-\frac{5}{3}} e^{\beta(1+\frac{2}{5}\delta^2)} \exp(-\beta(1+0.4\delta^2 k^2)k^{\frac{4}{3}}), \tag{6}$$

$$\text{where } \beta := \frac{3}{2}\frac{\nu\alpha}{\varepsilon_0^{1/3}}, \text{ and } \varepsilon_0 = 2^{-3/2}\alpha^{-1}U^3. \tag{7}$$

This gives (Section 4.1) that up to the wave number associated with the microscale $k = 1/\eta_{ADM}$ we have

$$E(k) \doteq \alpha\varepsilon^{2/3}k^{-5/3}, \text{ over } 1 < k < 1/\eta_{ADM}.$$

This is very accurate for smaller wave numbers (in the resolved frequencies $0 < k < 1/\delta$); for larger wave numbers, $1/\delta < k < 1/\eta_{ADM}$, exponential decay is not dominant but begins to bend the spectrum down, as expected.

The influence of time relaxation term is analyzed in Section 4.2. It is shown that a careful choice of the relaxation parameter can accelerate the dissipation range to begin at the transition point between resolved and unresolved scales: $\eta_{\text{model}} = \delta$.

In Section 5 we give numerical results from an upwind type discretization of the $\partial/\partial k(\cdot)$ term and the Runge Kutta 4th order routine, implemented in Matlab, for the time variable. Discretization of the $\partial/\partial k(\cdot)$ term thus results in a Pao-ADM shell model. Consistent with work on shell models we pick break points in wave number space by equi-distribution of model kinetic energy and give an estimate of the computational complexity of solving the resulting shell model using Runge Kutta 4th order algorithm. The resulting experiments in Section 5 fully corroborate the predictions in Section 4.

2. Reduction of the ADM (5) to simpler form

For each $N = 0, 1, ...$ the van Cittert deconvolution algorithm it computes an approximate filter inverse $u_N = D_N\overline{u} := \sum_{n=0}^{N}(I - A^{-1})^n\overline{u}$. $D_N\overline{u}$ is typically computed, [3], by N steps of the fixed point iteration: $u^{new} = u^{old} + \{\overline{u} - A^{-1}u^{old}\}$.

Algorithm 2.1 (van Cittert approximate deconvolution algorithm)**.** *Set* $u_0 = \overline{u}$*, For* $n = 1, 2, \cdots, N-1$*, perform:* $u_{n+1} = u_n + \{\overline{u} - A^{-1}u_n\}$.
Then $D_N\overline{u} := u_N$.

The zeroth order approximate deconvolution model (5), [16], and [21], arises when $N = 0$ and $\chi = 0$:

$$w_t + \nabla \cdot (\overline{w}\ \overline{w}) - \nu\triangle w + \nabla q = \overline{f}, \text{ and } \nabla \cdot w = 0. \tag{8}$$

Applying $A = -\delta^2 \triangle + I$ to (8) reduces it to an equivalent form with the same nonlinearity as the NSE (which is $\nabla \cdot (w\ w)$) with an extra hyperviscosity term $(\nu\delta^2 \triangle^2 w)$ and an extra kinetic energy term $(-\delta^2 \triangle w_t)$:

$$\left(w - \delta^2 \triangle w\right)_t + \nabla \cdot (w\ w) - \nu\triangle\left(w - \delta^2 \triangle w\right) + \nabla\widetilde{q} = f, \text{ and } \nabla \cdot w = 0.$$

Consider now the full ADM: $\nabla \cdot w = 0$ and

$$w_t + \nabla \cdot (\overline{D_N w}\ \overline{D_N w}) - \nu \triangle w + \nabla q + \chi\,(w - D_N \overline{w}) = \overline{f}.$$

Define a new filtering operator $H := D_N A^{-1}$ denoted by a tilde:

$$\widetilde{\phi} = H\phi := D_N \overline{\phi}.$$

Let $v := D_N w$. Since $w \simeq \overline{u}$, so $v = D_N(w) \simeq u$. Applying D_N reduces the full ADM to the zeroth order model for the new velocity v with a different filter and time relaxation: $\nabla \cdot v = 0$ and

$$v_t + \nabla \cdot (\widetilde{v\ v}) - \nu \triangle v + \nabla q + \chi\,(v - Hv) = Hf.$$

Adapting the simplification of the zeroth order model's nonlinear term for the full ADM, apply H^{-1} to this equation, giving $\nabla \cdot v = 0$, and

$$H^{-1} v_t + \nabla \cdot (v\ v) - \nu \triangle H^{-1} v + \nabla q + \chi\,(H^{-1} v - v) = f. \tag{9}$$

This derived equation is related to the original ADM by an invertible change of variables. It has the same nonlinearity as the NSE and thus the Pao energy transfer theory can be applied directly to its nonlinear term without any alteration or adaptation.

3. Pao's Transfer Theory applied to the ADM

Consider the transformed form of the full ADM (9) in a three dimensional 2π periodic box. Under periodicity, the fluid velocity and its associated kinetic energy can be expanded in Fourier series (in the sums $\mathbf{k} \neq (0,0,0)$[1])

$$v(x,t) = \sum_{\mathbf{k}} \widehat{v}(\mathbf{k},t) e^{i\mathbf{k}\cdot x}, \ \text{ and } \ E(t) = \sum_{\mathbf{k}} \frac{1}{2} |\widehat{v}(\mathbf{k},t)|^2.$$

Transfer theory is based on a partition of the kinetic energy into wave number shells given by Fourier series follows. Define $|\mathbf{k}|^2 = k_1^2 + k_2^2 + k_3^2$ and

$$E(k,t) := \sum_{k=|\mathbf{k}|} \frac{1}{2} |\widehat{v}(\mathbf{k},t)|^2, \ \text{so that } E(t) = \sum_{1 \leq \mathbf{k}} E(k,t).$$

In this definition of $E(k,t)$, the index k in the sum takes non integer values (e.g., $\mathbf{k} = (1,1,1)$, $k = \sqrt{3}$). This will be no difficulty since transfer theories are further approximations in which k will (in the end) be a continuous variable. Further, $E(k,t)$ represents the energy in $v := D_N w$. Since $w \simeq \overline{u}$, so $v = D_N(w) \simeq u$. Thus, $E(k,t)$ is an approximation to the energy in u and not in $\overline{u}$.

Exact but non closed equations for $E(k,t)$ are derived in the usual way by taking the inner product of the equations (9) with one Fourier mode and then summing over $|\mathbf{k}| = k$, see Davidson [7], Frisch [10], or Pope [26] for details. Suppressing the dependence on N, let[2] $h(k) := \widehat{H^{-1}}(k)$. This gives (using the Kronecker delta)

$$h(k) \frac{\partial}{\partial t} E(k,t) + \sum_{|\mathbf{j}|=k} \sum_{\mathbf{k}_1} \sum_{\mathbf{k}_2} \left\{ \widehat{v}(\mathbf{k}_1,t) \cdot \widehat{v}(\mathbf{k}_2,t) \otimes \mathbf{k}_2 \cdot \overline{\widehat{v}(\mathbf{j},t)} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{j}} \right\} +$$
$$+ 2\nu k^2 h(k) E(k,t) + \chi\,(h(k) - 1)\, E(k,t) = \sum_{|\mathbf{j}|=k} \widehat{f}(\mathbf{j},t) \cdot \overline{\widehat{v}(\mathbf{j},t)}.$$

[1] Further, since $\nabla \cdot u = 0$ and u is real, $\mathbf{k} \cdot \widehat{u}(\mathbf{k},t) = 0$ and $\widehat{u}(\mathbf{k},t) = \overline{\widehat{u}(-\mathbf{k},t)}$.

[2] For example, when $N = 0$, $h(k) = (\widehat{D_0 A^{-1}})(k) = \left(I\,(-\delta^2 \widehat{\triangle} + I)^{-1} \right)(k) = \left(\delta^2\, k^2 + 1\right)^{-1}$

Define $T(k,t)$ and the *energy transfer function* $S(k,t)$:

$$\begin{aligned} T(k,t) &:= \sum_{|\mathbf{j}|=k} \sum_{\mathbf{k}_1} \sum_{\mathbf{k}_2} \left\{ \widehat{v}(\mathbf{k}_1,t) \cdot \widehat{v}(\mathbf{k}_2,t) \otimes \mathbf{k}_2 \cdot \overline{\widehat{v}(\mathbf{j},t)} \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{j}} \right\} \\ S(k,t) &:= \sum_{1 \le k' \le k} T(k',t). \end{aligned}$$

The case of fully developed, homogeneous, isotropic turbulence corresponds to (i) smooth, persistent body forces, (ii) time averaged behavior of $E(k,t)$, and (iii) high Reynolds number with a richness of persistent scales of motion. Exploiting (iii), k is treated as a continuous variable; following (ii), we study time averages of $E(k,t)$ given by

$$E(k) := \lim_{T\to\infty} \frac{1}{T} \int_0^T E(k,t)dt\,, \tag{10}$$

and, motivated by (i), energy is input into the $k=1$ modes: $E(1,t) = \frac{1}{2}U^2,$ for all $t > 0$, where U is fixed.

To extend k to a continuous variable, sums are replaced by integrals in the usual way. Thus the *energy transfer function* $S(k,t)$ and the *energy* $E(k,t)$ satisfy, for fixed $U > 0$,

$$S(k,t) = -\int_0^k T(k',t)dk' \text{ or } S(k,t) = \int_k^\infty T(k',t)dk' \tag{11}$$

$$T(k,t) = \frac{\partial}{\partial k} S(k,t), \text{ and } E(1,t) = \frac{1}{2}U^2, \text{ for all } t > 0. \tag{12}$$

Remark 3.1. *Because of the change of variables in Section 2, the terms $E(k,t)$, $T(k,t)$ and $S(k,t)$ are defined exactly as for the Navier-Stokes equations. This means the correct extension of Pao's transport theory to the ADM (after the change of variables) is exactly the same closure in wave-number space as Pao used for the NSE.*

With these approximations we have the following (non-closed) energy equation:

$$h(k)\frac{\partial}{\partial t}E(k,t) + \frac{\partial}{\partial k}S(k,t) + \left(h(k)2\nu k^2 + \chi\left(h(k)-1\right)\right)E(k,t) = 0,$$

subject to $E(1,t) = 1/2U^2$, for $t > 0$, and $E(k,0) = E_0(k)$ where $E_0(k) \equiv 0$ for large k. A transfer theory is simply a closure which relates $S(k,t)$ back to $E(k,t)$ either through an algebraic relation (simplest) or an extra set of integro-differential equations, [7]. The goal of transfer theory is to develop a closed system of differential equations for $E(k,t)$ which is of much reduced complexity than the NSE in wave number space and predicts statistics of fully developed turbulence correctly. Energy transfer theories arose from the early work of Obukhov, Heisenberg, Onsager and others, see, e.g., [24], [7], [29]. The simplest and (so far) most successful is Pao [25], which generalizes Onsager's spectral jump condition, [23], in a simple and effective manner, postulating the algebraic relation $S(k,t) = \sigma E(k,t)$, $\sigma(\varepsilon,k) =$ proportionality constant. Equating units gives $\sigma = \alpha^{-1}\varepsilon_0^{1/3}k^{5/3}$ and the unique closure

$$S(k,t) = \alpha^{-1}\varepsilon_0^{1/3}k^{5/3}E(k,t), \text{ where } \varepsilon_0 = 2^{-3/2}\alpha^{-1}U^3. \tag{13}$$

Here α is the Kolmogorov constant (with value between 1.4 and 1.6) and ε_0 is the Pao model's energy dissipation rate. In justification, Y.-H. Pao writes (page 1067 in [25]):

> *"We visualize the transfer of turbulent energy as a cascading process in which the spectral elements are continuously transferred to even larger wave numbers.... Let the rate at which an energy spectral element is transferred across k be σ ... then the energy flux across k is $S(k) = E(k)\sigma(k)$. We assert that the spectral element $\sigma(k)$ is dependent on ε ... and on the wave number k .... Dimensional reasoning gives $\sigma(k) = \alpha^{-1}\varepsilon^{1/3}k^{5/3}$."*

We study the long time averaged behavior of solutions to the following hyperbolic, initial boundary value problem with time relaxation damping:

$$\begin{gathered} h(k)\frac{\partial}{\partial t}E(k,t) + \frac{\partial}{\partial k}(\alpha^{-1}\varepsilon_0^{1/3}k^{5/3}E(k,t)) + \left(h(k)2\nu k^2 + \chi\left(h(k)-1\right)\right)E(k,t) = 0, \\ \text{for } 1 < k < \infty, t > 0, \\ E(1,t) = \frac{1}{2}U^2, \text{ for } t > 0, \text{ and } \varepsilon_0 = 2^{-3/2}\alpha^{-1}U^3, \\ E(k,0) = E_0(k) \text{ for } 1 < k < \infty \text{ where } E_0(k) \equiv 0 \text{ for large } k. \end{gathered} \tag{14}$$

The characteristics of (14) are non-intersecting and positive sloped curves given by

$$h(k)dt - \frac{5}{3}\alpha^{-1}\varepsilon_0^{1/3}k^{5/3}dk = 0.$$

The problem (14) reduces to a linear ordinary differential equation along each characteristic. From this existence and uniqueness follows immediately from standard theory of hyperbolic equations, [33].

Proposition 3.2. *Let $E_0(k) \equiv 0$ for large k. A unique solution exists to problem (14). For each fixed $t > 0$ the solution $E(k,t)$ has compact support in k.*

The energy input defines a clear representative large scale velocity U. The natural large length scale is $L = 2\pi$. Thus, the natural Reynolds number associated with the Pao energy transfer model is

$$Re = \frac{|nonlinearity|}{|viscous\ term|} = \frac{U\frac{1}{2\pi}U}{\nu\left(1+\left(\frac{\delta}{2\pi}\right)^2\right)\frac{1}{(2\pi)^2}U} \doteq 2\pi\frac{U}{\nu} \text{ since } \delta \text{ is small.}$$

The long time averaged energy distribution is defined to be

$$E(k) = \lim_{T\to\infty}\frac{1}{T}\int_0^T E(k,t)dt.$$

This limit exists (Corollary 4.2 below). Its value is determined by the properties of the equilibrium problem associated with (14), given by $E_\infty(1) = \frac{1}{2}U^2$ and

$$\frac{\partial}{\partial k}(\alpha^{-1}\varepsilon_0^{1/3}k^{5/3}E_\infty(k)) + \left(h(k)2\nu k^2 + \chi\left(h(k)-1\right)\right)E_\infty(k) = 0. \tag{15}$$

The equilibrium Pao-ADM is easily seen to have a unique solution. It has exponential decay for large k and, (when $N = 0, \chi = 0$) is given by

$$E_\infty(k) = \frac{1}{2}U^2k^{-\frac{5}{3}}e^{\beta(1+0.4\delta^2)}\exp(-\beta(1+0.4\delta^2k^2)k^{\frac{4}{3}}), \quad \text{where} \quad \beta := \frac{3}{2}\frac{\nu\alpha}{\varepsilon_0^{1/3}}.$$

4. Analysis of Pao's Transfer Theory for ADMs

The goal of energy transfer theory is to develop a single and consistent phenomenology that explains the K41 theory as well as giving insight into the transition between $k^{-5/3}$ in the inertial range and exponential decay in the dissipation range, including:

- statistical equilibrium: energy input at large scales balanced by energy dissipation at small scales.
- $k^{-5/3}$ energy spectrum through the inertial range transitioning to exponential decay in the dissipation range.
- an estimate of the microscale between inertial and dissipation ranges.

First we analyze the predictions of these features for the ADM transfer model without time relaxation (i.e. $\chi = 0$ case) and, following this, the effect of time relaxation.

Proposition 4.1. *Let $\chi \geq 0$ and let $E(k,t)$, $E_\infty(k)$ denote respectively the solutions to (14) and (15). Then $E(k,t) \to E_\infty(k)$ exponentially fast in $L^2(1,\infty)$ as $t \to \infty$, (even in the case $\nu = \chi = 0$).*

Proof. We give the proof in the notationally simplest $N = 0$ case. The proof for $N > 0$ is the same only notationally more complex. Let $e(x,t) = E(k,t) - E_\infty(k)$. Since $E(k,t)$ has compact support, $e(k,t)$ decreases exponentially in k (and thus all integrals below are convergent). Subtraction gives the following equation for $e(k,t) : e(1,t) = 0$, for $t > 0$, and $e(k,0)$ given and

$$(1+\delta^2k^2)\frac{\partial}{\partial t}e(k,t)+\frac{\partial}{\partial k}(\alpha^{-1}\varepsilon_0^{1/3}k^{5/3}e(k,t))+\left(2\nu(1+\delta^2k^2)k^2+\chi\delta^2k^2\right)e(k,t)=0.$$

Multiply by $e(k,t)$ and integrate. This yields

$$\frac{d}{dt}\int_1^\infty \frac{1}{2}(1+\delta^2k^2)e(k,t)^2dk+$$
$$+\int_1^\infty \left[\frac{5}{6}\alpha^{-1}\varepsilon_0^{1/3}k^{5/3}+2\nu(1+\delta^2k^2)k^2+\chi\delta^2k^2\right]e(k,t)^2dk=0.$$

The term in brackets is bounded below by $5/6\alpha^{-1}\varepsilon_0^{1/3}$, a positive constant, even if $\nu = \chi = 0$. Thus, we have exponential convergence to steady state.

Thus, $E(k,t)$ approaches the unique solution of the equilibrium problem as $t \to \infty$, $E_\infty(k) = E(k)$ given by

$$E(k) = \frac{1}{2}U^2k^{-\frac{5}{3}}e^{\beta(1+0.4\delta^2)}\exp(-\beta(1+0.4\delta^2k^2)k^{\frac{4}{3}}), \text{ where } \beta := \frac{3}{2}\frac{\nu\alpha}{\varepsilon_0^{1/3}}. \tag{16}$$

The fact that exponential convergence to a $k^{-5/3}$ energy spectrum occurs even for the $\nu = \chi = 0$ ADM energy transfer model is perhaps relevant to the Onsager conjecture that "*... in three dimensions a mechanism for complete dissipation of all kinetic energy, even without the aid of viscosity, is available,*"(L. Onsager, 1949). From the last proposition and following arguments in [22], it follows that time averages on $E(k,t)$ exist and correspond to the equilibrium solution.

Corollary 4.2. *Let $E(k,t)$, $E_\infty(k)$ denote respectively the solutions to (14) and (15). The following limit exists and equals:*

$$E(k) := \lim_{T\to\infty}\frac{1}{T}\int_0^T E(k,t)dt = E_\infty(k).$$

Thus, we may check predictions of the Pao transfer theory through (16). The formula for the equilibrium solution reveals that there are two wave number regimes: resolved scales and unresolved scales.

Inertial Range: If $\beta(1+0.4\delta^2k^2)k^{\frac{4}{3}} << 1$, then $E(k) \doteq \frac{1}{2}U^2k^{-\frac{5}{3}}$. Over the subrange of resolved scales $(1 \leq k \leq 1/\delta)$ where $(1+0.4\delta^2k^2) \simeq 1$, $E(k)$ replicates the NSE's Pao spectrum

$$E(k) \doteq \frac{1}{2}U^2k^{-\frac{5}{3}}e^{\beta}\exp(-\beta k^{\frac{4}{3}}) \text{ for } k < 1/\delta. \tag{17}$$

Dissipation Range: If $\beta(1+0.4\delta^2k^2)k^{\frac{4}{3}} \geq 1$, the solution exhibits accelerated energy decay

$$E(k) \doteq \frac{1}{2}U^2k^{-\frac{5}{3}}e^{C(\delta)\beta}\exp(-\beta\delta^2k^{\frac{10}{3}}). \tag{18}$$

4.1. Consistency with the K41 Theory. We now turn to consistency of the predictions with Kolmogorov's theory of homogeneous, isotropic turbulence checking predictions of statistical equilibrium, the inertial energy range spectrum, exponential decay in the dissipation range and the predicted microscale. With $\varepsilon_0 = 2^{-3/2}\alpha^{-1}U^3$, consider the Pao ADM's energy spectrum given by (16).

Statistical equilibrium. Statistical equilibrium in the K41 theory means that the energy input to the large scales (which is $O(U^3/L)$) is balanced (after time averaging) by energy dissipation primarily at the small scales. When $\chi = 0$ the time averaged energy dissipation rate of (14) is given by

$$\varepsilon_{ADM} := \lim_{T\to\infty}\frac{1}{T}\int_0^T\int_1^\infty 2\nu(1+\delta^2k^2)k^2E(k,t)dkdt$$

We calculate directly that as $\delta \to 0, \varepsilon_{ADM} \to \varepsilon_0$ which is exactly the time averaged energy dissipation rate predicted for the NSE by the Pao model. Indeed,

$$\begin{aligned}
\varepsilon_{ADM} := & \lim_{T\to\infty}\frac{1}{T}\int_0^T\int_1^\infty 2\nu(1+\delta^2k^2)k^2E(k,t)dkdt \\
= & \int_1^\infty 2\nu(1+\delta^2k^2)k^2E_\infty(k)dk \\
= & \nu U^2e^{\beta(1+0.4\delta^2)}\int_1^\infty(1+\delta^2k^2)k^{\frac{1}{3}}\exp(-\beta(1+0.4\delta^2k^2)k^{\frac{4}{3}})dk \\
\to & \nu U^2e^{\beta}\int_1^\infty k^{\frac{1}{3}}\exp(-\beta k^{\frac{4}{3}})dk = \varepsilon_0
\end{aligned}$$

Surprisingly, the relation $\varepsilon_{ADM} = Const.\varepsilon_0$ holds exactly, not just asymptotically. Indeed, integrating (14) and time averaging gives

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T\int_1^\infty(1+\delta^2k^2)E_t(k,t)+$$
$$+(\alpha^{-1}\varepsilon_0^{1/3}k^{5/3}E(k,t))_k + 2\nu(1+\delta^2k^2)k^2E(k,t)dkdt = 0.$$

Using Fubini's theorem, the first term vanishes and the time average of the third term is exactly ε_{ADM}. We then have from the second term, that $E_\infty(k) \to 0$ as $k \to \infty$, the boundary condition at $k = 1$ and the third term $\alpha^{-1}\varepsilon_0^{1/3}\frac{1}{2}U^2 = \varepsilon_{ADM}$. The Pao model for the NSE predicts that $\varepsilon_0 = CU^3$ (since $L = 2\pi$). Thus, in the last equation $U^2 = \left(U^3\right)^{2/3} = C\varepsilon_0^{2/3}$ and, as required for statistical equilibrium, $\varepsilon_{ADM} = C\varepsilon_0$.

The inertial range energy spectrum. Since $E(k,t)$ is bounded, and $Re = 2\pi U/\nu$ is large, there is a range of k ($1 < k < 1/\eta_{ADM}$, say) for which the term $2\nu(1+\delta^2k^2)k^2E(k,t)$ is negligible. On this range, (14) simplifies to

$$(1+\delta^2k^2)E_t(k,t) + (\alpha^{-1}\varepsilon_0^{1/3}k^{5/3}E(k,t))_k \doteq 0.$$

Integrating over $1 < k' < k$ ($< 1/\eta_{ADM}$), time averaging and using Fubini's theorem, the term $(1+\delta^2k^2)E_t(k,t)$ drops out and we have

$$\int_1^k (\alpha^{-1}\varepsilon_0^{1/3}k'^{5/3}E(k'))_{k'}dk' \doteq 0, \text{or } \alpha^{-1}\varepsilon_0^{1/3}k^{5/3}E(k) \doteq \alpha^{-1}\varepsilon_0^{1/3}\frac{1}{2}U^2.$$

From the choice of ε_0, $\frac{1}{2}U^2 = \alpha\varepsilon_0^{2/3}$. Thus, rearranging

$$E(k) \doteq \alpha\varepsilon^{2/3}k^{-5/3}, \text{ over } 1 < k < 1/\eta_{ADM}.$$

The dissipation range. The K41 theory predicts exponential decay in $E(k)$ for large k and gives an estimate of the microscale at which this decay begins to be the dominant effect. Exponential decay of $E(k)$ follows immediately for k large enough that exponent $\beta(1+\frac{2}{5}\delta^2k^2)k^{\frac{4}{3}}$ is $O(1)$ or larger from (16). The transition point / microscale is calculable since $\beta := 3\nu\alpha/(2\varepsilon^{1/3})$, and $\varepsilon = 2^{-3/2}\alpha^{-1}U^3$. Indeed, the exponent $\beta(1+\frac{2}{5}\delta^2k^2)k^{\frac{4}{3}}$ is $O(1)$ or larger when

$$\nu U^{-1}(1+\frac{2}{5}\delta^2k^2)k^{4/3} = O(1).$$

This equation determines the Pao-ADM transition model's microscale. There are two cases depending on which term, 1 or $\frac{2}{5}\delta^2k^2$, is dominant.

Case 1: If the averaging radius δ is $O(\eta_{NSE})$ or smaller, where $\eta_{NSE} \doteq Re^{-3/4}L$ is the Kolmogorov microscale of the NSE. This is the case of a fully resolved flow and is of less interest than case 2. Case 1 corresponds to $\delta^2k^2 \ll O(1)$, so that $(1+2/5\delta^2k^2) \simeq 1$. The condition $\nu U^{-1}(1+\frac{2}{5}\delta^2k^2)k^{4/3} = O(1)$ becomes $\nu U^{-1}k^{4/3} = O(1)$. This implies (after rearrangement) $k \doteq (U/\nu)^{3/4} \doteq Re^{3/4}/L$, as $L = 2\pi$ yielding the predicted models's microscale of

$$\eta_{ADM} = \eta_{NSE} \doteq Re^{-3/4}L, \text{ when } \delta \leq O(\eta_{NSE}).$$

Case 2: If $\delta >> O(\eta_{NSE})$. This is the typical case of under-resolved flow. Case 2 corresponds to $\delta^2k^2 >> O(1)$, so that $(1+2/5\delta^2k^2) \simeq 2/5\delta^2k^2$. The condition $\nu U^{-1}(1+\frac{2}{5}\delta^2k^2)k^{4/3} = O(1)$ becomes $\nu U^{-1}\delta^2k^{10/3} = O(1)$. This implies (after rearrangement) $k \doteq \left(\nu U^{-1}\delta^2\right)^{-3/10}$ yielding the models' microscale of

$$\eta_{ADM} \doteq Re^{-3/10}\delta^{3/5}L, \text{ when } \delta >> O(\eta_{NSE})$$

which agrees with the result derived using direct application of turbulence phenomenology to the ADM in [20].

4.2. Influence of time relaxation. Since time relaxation, the case $\chi > 0$, dissipates energy in all cases, its main issue is the choice of the (user supplied) parameter χ. We pick χ to enforce $\eta_{ADM} = \delta$. For deconvolution order $N = 0$ and $\chi > 0$ the equilibrium energy distribution satisfies

$$\frac{\partial}{\partial k}(\alpha^{-1}\varepsilon_0^{1/3}k^{5/3}E(k)) + 2\nu k^2\left(1+\frac{\chi\delta^2}{2\nu}+\delta^2k^2\right)E(k) = 0 \ , E(1) = \frac{1}{2}U^2 \tag{19}$$

With $\beta := 3\nu\alpha/(2\varepsilon^{1/3})$, and $\varepsilon = 2^{-3/2}\alpha^{-1}U^3$, we find

$$E(k) = \alpha\varepsilon^{2/3}k^{-\frac{5}{3}}e^{\beta(1+\frac{2}{5}+\delta^2\frac{\chi\delta^2}{2\nu})}\exp(-\beta(1+\frac{2}{5}\delta^2k^2+\frac{\chi\delta^2}{2\nu})k^{\frac{4}{3}}).$$

Thus, increasing χ increases the multiplier in the exponent from $(1+\frac{2}{5}\delta^2k^2)$ to $(1+\frac{2}{5}\delta^2k^2+\frac{\chi\delta^2}{2\nu})$. This increases energy decay in the dissipation range and the model microscale where exponential decay begins to be significant.

Set the microscale $\eta_{ADM} = \delta$ and solve for the induced χ value. Exponential decay becomes significant where $\beta(1+\frac{2}{5}\delta^2k^2+\frac{\chi\delta^2}{2\nu})k^{\frac{4}{3}} = O(1)$. If $\eta_{ADM} = \delta$ then $\delta^2k^2 = 1$ and this reduces to $\beta(7/5+\chi\delta^2/(2\nu))\delta^{-\frac{4}{3}} \doteq 1$. Solving for χ recovers the formula of [19]:

$$\chi = \left(\frac{4}{3}\varepsilon^{1/3}\alpha^{-1}\right)\delta^{-2/3} - \left(\frac{7\pi}{5}U\right)\mathrm{Re}^{-1}\delta^{-2}. \tag{20}$$

Calculating the crossover point in the two terms on the RHS we find that $\chi > 0$ provided $\frac{\delta}{L} > \mathrm{Re}^{-3/4} = \eta_{NSE}$, which is exactly as desired: the extra dissipation induced by time relaxation under the formula (20) decreases to zero as the LES approaches a DNS.

5. Numerical Tests of the Pao-ADM Shell Model

Shell models are low dimensional dynamical systems descriptions of the time evolution of the energy in wave number shells in turbulent flows, e.g., [8], [6]. When the wave number in (14) is discretized a shell model results. The energy in the m^{th} wave number shell is denoted herein by $E_m(t)$ (and often elsewhere by $u_m(t)$). Given wave number levels k_m and associated energy shell levels $E_m(t), m = 1, 2, ..., M$,upwind difference the $\partial/\partial k$ term in (14). This gives the following Pao-ADM shell model: $E_1(t) = \frac{1}{2}U^2$ and for $m = 2, \cdots, M$,

$$(1+\delta^2k_m^2)\frac{\partial}{\partial t}E_m(t) + \alpha^{-1}\varepsilon_0^{1/3}\left(\frac{k_m^{5/3}E_m(t) - k_{m-1}^{5/3}E_{m-1}(t)}{k_m - k_{m-1}}\right) + \\ +2\nu(1+\delta^2k_m^2)k_m^2E_m(t) = 0. \tag{21}$$

5.1. Choice of shell levels by equi-distribution of energy. The energy spectrum of the transformed ADM solution v (which approximates u not $\overline{u}$) is approximately $\alpha\varepsilon_0^{2/3}k^{-5/3}$ over $1 \le k \le 1/\eta_{ADM}$. Thus the energy spectrum of the untransformed ADM solution w is approximately $\alpha\varepsilon_0^{2/3}k^{-5/3}$. We have selected energy levels by equi-distribution of the untransformed energy distribution. The total kinetic energy (up to exponentially small terms) is

$$TotalEnergy := \int_1^{1/\eta_{ADM}} E(k)dk \doteq \int_1^{1/\eta_{ADM}} \alpha\varepsilon_0^{2/3}k^{-5/3}dk = \frac{3}{2}\alpha\varepsilon_0^{2/3}(1-\eta_{model}^{2/3}).$$

The M shell levels $k_m, m = 1, \cdots, M$, are chosen to equi-distribute the $TotalEnergy$ by

$$\begin{aligned} k_1 &= 1, \\ k_{m+1}^{-2/3} &= k_m^{-2/3} - \frac{2\cdot TotalEnergy}{3M}, \text{ for } 1 \le k_m \le 1/\eta_{ADM}, \\ k_M &= 1/\eta_{model}. \end{aligned} \tag{22}$$

5.2. Complexity of the Runge Kutta 4th order Algorithm. The shell model (21) was solved using Runge Kutta 4th order routine implemented in Matlab, (whose complexity is estimated next), until statistical equilibrium (in all cases by $T_{final} = 30$). With timestep $\triangle t$, the resulting complexity is roughly

$$Complexity = M \times (\#FLOPs/eqn) \times (T_{final}/\triangle t)$$

The implemented Runge Kutta routine requires about 20 floating point operations to evaluate the nonlinearity in (21) per stage per equation. Computing the $E_m(t^{n+1})$ after 4 stages requires eight additional operations, yielding

$$Complexity \doteq 88M\frac{T_{final}}{\Delta t} \tag{23}$$

Since the shell model is a discretized hyperbolic equation, we halved the time step $\triangle t$ until the usual CFL condition (below) is satisfied

$$\max_{m=1,\cdots,M} \frac{\alpha^{-1}\varepsilon_0^{1/3}k_m^{5/3}}{(1+\delta^2 k_m^2)}\frac{\Delta t}{k_m - k_{m-1}} < 1.$$

By the stopping process of halving $\triangle t$ upon satisfaction of the CFL condition, we also enforced a lower bound and thus the following two sided bounds

$$\begin{aligned} &\frac{\alpha\varepsilon_0^{-1/3}}{2}\min_{m=1,\cdots,M} k_m^{-5/3}(1+\delta^2 k_m^2)(k_m - k_{m-1}) < \Delta t, \text{ and} \\ &\Delta t < \alpha\varepsilon_0^{-1/3}\min_{m=1,\cdots,M} k_m^{-5/3}(1+\delta^2 k_m^2)(k_m - k_{m-1}). \end{aligned} \tag{24}$$

Lemma 5.1. *With k_m and Δt chosen as above, we have*

$$k_m^{-5/3}\,(k_{m+1} - k_m) \;>\; \frac{TotalEnergy}{U^2 M}, \quad for \;\; m = 1, 2, \cdots, M, \tag{25}$$

$$\Delta t \;>\; \frac{\sqrt{2}}{4}\alpha^{4/3}\frac{TotalEnergy(1+\delta^2)}{U^3 M}. \tag{26}$$

Proof. The mean value theorem on $[k_m, k_{m+1}]$ with $g(k) = k^{-2/3}$ gives, for $\xi \in (k_m, k_{m+1})$,

$$(-\frac{2}{3}\xi^{-5/3}) \cdot (k_{m+1} - k_m) = -\frac{2}{3}\frac{TotalEnergy}{U^2 M},$$

Since $\xi \mapsto \xi^{-5/3}$ is decreasing, this yields the claimed result:

$$k_{m+1} - k_m = \frac{TotalEnergy \cdot \xi^{5/3}}{U^2 M} \geq \frac{TotalEnergy \cdot k_m^{5/3}}{U^2 M}.$$

Consider now the lower bound upon $\triangle t$ in (24). From the first bound in the lemma,

$$k_m^{-5/3}(1+\delta^2 k_m^2)\,(k_{m+1} - k_m) > \frac{TotalEnergy\,(1+\delta^2 k_m^2)}{U^2 M}.$$

Thus, since $1 + \delta^2 k_m^2 \geq 1 + \delta^2$ and $k_m^{-5/3}\,(k_{m+1} - k_m) > TotalEnergy/U^2 M$, we have

$$\Delta t > \frac{\alpha\varepsilon_0^{-1/3}TotalEnergy(1+\delta^2)}{2U^2 M}.$$

Using $\varepsilon_0 = 2^{-3/2}\alpha^{-1}U^3$, we conclude

$$\Delta t > \frac{\sqrt{2}}{4}\alpha^{4/3}\frac{TotalEnergy(1+\delta^2)}{U^3 M}.$$

■

Using this lower bound on Δt in (23) and the other estimates for the various terms and simplifying yields the following.

Proposition 5.2 (Complexity of Solving the Pao Shell Model)**.** *Under the time step condition (24) solving (21) with Runge Kutta 4th order routine, requires complexity (measured in floating point operations) of the order*

$$Complexity \leq \frac{352\sqrt{2}}{3}\alpha^{-2/3}UM^2T_{final}.$$

5.3. Results. The Pao-ADM shell model displayed the behavior of the time averaged solutions to (21) for the number M of shell levels moderate. The computed energy distribution agreed with predictions over the full range $1 \leq k \leq 1/\eta_{model}$. Indeed, Figure 1 shows a clear $k^{-5/3}$ energy spectrum over $1 \leq k \leq 1/\delta$ (and a bit beyond even). Over $1/\delta << k \leq 1/\eta_{model}$ there is a smooth and gradual transition to exponential decay. We see no evidence of a secondary $k^{-11/3}$ decay over $1/\delta \leq k \leq 1/\eta_{model}$ in $E(k)$. (Compare the dotted curve against the line segments depicting both slopes.) Since the energy in w is related to that computed, $E(k)$, by

$$Energy(w) \simeq E(k)/(1+\delta^2k^2)$$

a $k^{-5/3}$ spectrum in $E(k)$ is clear evidence of a secondary $k^{-11/3}$ decay over $1/\delta \leq k \leq 1/\eta_{model}$ in the energy in w, as predicted in [20]. Since the question can arise if the observed energy spectrum was somehow built in by the selected equi-distribution principle, we also repeated this calculation but selecting k_n instead by equi-distribution of $E(k)/(1+\delta^2k^2)$. The spectrums computed for $E(k)$ (not plotted herein) with different shell levels did not change.

Figure 1 gives a logarithmic plot of the time average of $E_n(t)$ in a model simulation with $M = 200$ wave numbers with $\delta = 0.7$ chosen to have 100 shells in each range, $1 \leq k \leq 1/\delta$ and $1/\delta \leq k \leq 1/\eta_{model}$.

Correct predictions depended upon having a large enough number of shell levels. A test with almost identical initial conditions, $\delta = 0.6$ and of only $M = 50$ shells fails to produce the dissipation range, Figure 2.

6. Conclusions

The Pao energy transfer model is the simplest and the most successful transfer theory in that it predicts the major statistics of isotropic turbulence successfully. The Pao energy transfer analysis of ADMs recovers the correct $k^{-5/3}$ energy spectrum and the increase of the ADM microscale. Transfer theory also gives a formula for relaxation parameter selection induced by perfect resolution agreeing with one derived through similarity. Thus, transfer theory indicates strongly that ADMs capture essential, universal features of turbulence accurately and without special adjustments.

Energy transfer models other than the Pao model generally fail to predict turbulence statistics correctly. On the other hand, the Pao model can be criticized for being too successful: as t increases $E(k,t)$ converges smoothly and rapidly to the correct statistical energy distribution. For example, the Pao theory predicts that the ADM energy spectrum $E(k,t)$ approaches its time averaged value exponentially fast. Thus the Pao model does not capture time dependent behavior, such as energy bottlenecks and intermittence, of turbulence. One major open question in the Pao theory is thus how to extend Pao based energy transfer models and derived shell models so as to capture effects reminiscent of intermittence.

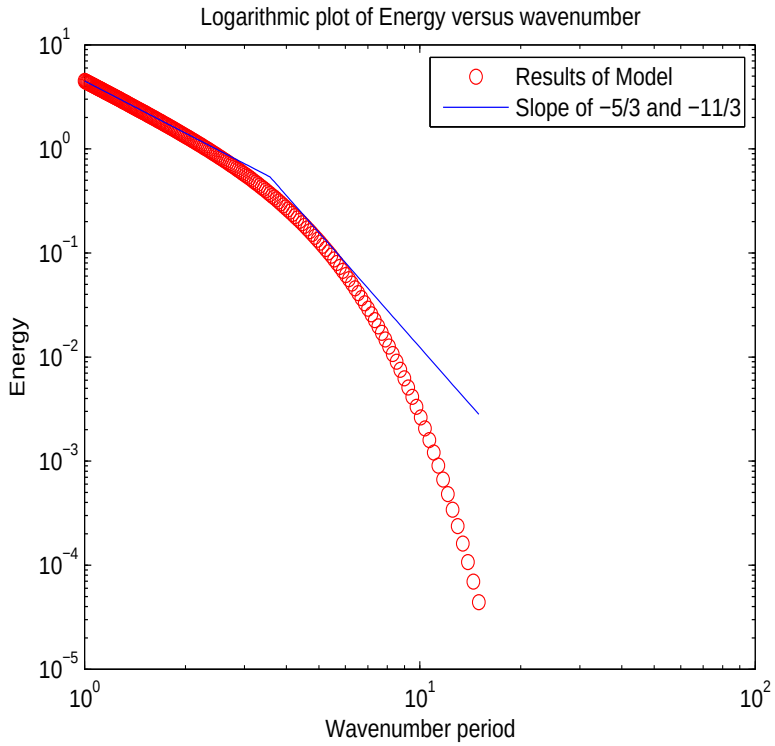

FIGURE 1. Energy spectrum with $M = 200$.

Acknowledgments

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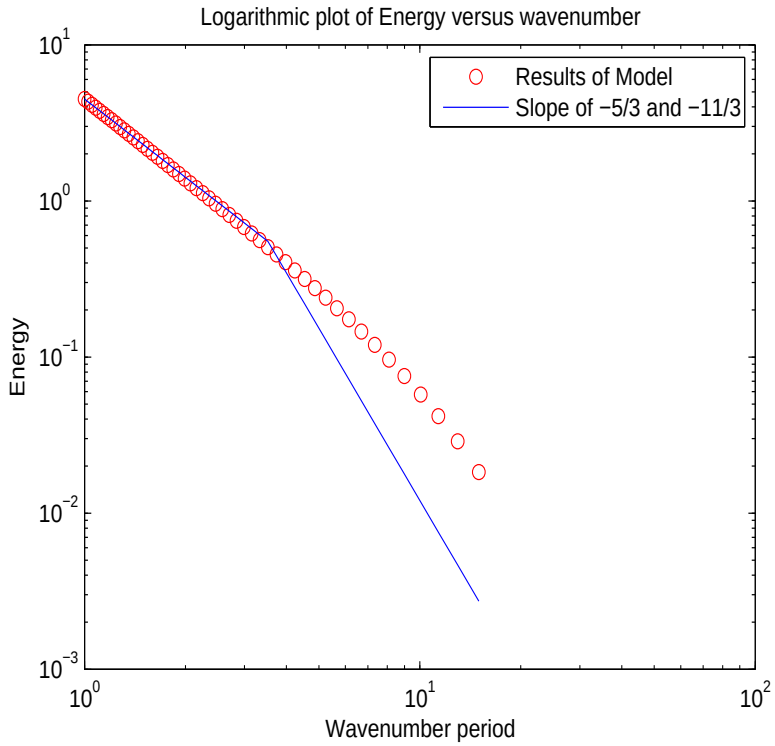

FIGURE 2. Energy spectrum with $M = 50$.

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