OPTIMIZATION AND CONTROL THEORY IN SHELL MODELS OF TURBULENCE

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Abstract

In this article, we present preliminary work on the development of a theoretical methodology based on optimization schemes and on optimal and control approaches in order to optimize and control the forcing of turbulence, and we applied this methodology to the Obukhov and Gledzer-Okhitani-Yamada shell models.

Key words

Turbulence, Shell Models, Optimization, Optimal Control.

1 Introduction

Shell models of turbulence were introduced by Obukhov and Gledzer (see [Obukhov, 1971; Gledzer, 1973; Ditlevsen, 2007]). The original purpose was to find a particular closure scheme which is able to reproduce the Kolmogorov spectrum, [Kolmogorov, 1941a; Kolmogorov, 1941b; Kolmogorov, 1941c], in terms of an attractive fixed point of an appropriate set of differential equations for the velocity field averaged over shells in Fourier space, while mimicking the Navier-Stokes equations, in the sense of preserving some invariants, by a dynamical system of dimension N, say, in the complex-valued time-dependent variables $u_1(\cdot), u_2(\cdot), \cdots, u_N(\cdot)$, each representing the typical magnitude of the velocity field on a certain length scale.

These models consist of a set of coupled nonlinear ordinary differential equations structurally similar to the Navier-Stokes equation written in the Fourier space, but are much simpler, and numerically easier, to investigate than the original Navier-Stokes equations. For these models a scaling theory identical to the Kolmogorov theory, [Kolmogorov, 1941a; Kolmogorov, 1941b; Kolmogorov, 1941c], has been developed, and they show the same kind of deviation from the Kolmogorov scaling as real turbulent systems do. Understanding the behavior of shell models in their own right is one of the keys to understand the systems governed by the Navier-Stokes equations. The shell models are constructed to obey the same conservation laws and symmetries as the Navier-Stokes equations.

In this article, we develop a theoretical methodology based on optimal and control approach in order to optimize and control the forcing of turbulence, and discuss their application to the Obukhov and Gledzer-Okhitani-Yamada shell models. The goal is to tune the force so that a given cost functional is minimized. Following the ideas of [Farazmand *et al.*, 2011], we want to reach the statistical regime observed in the structure functions within a certain given and fixed time interval $[0, T]$.

This article is organized as follows. In Sections 2 and 3, we present, respectively, the Obukhov and Gledzer-Okhitani-Yamada (GOY) models. The ensuing section is devoted to the mathematical formulation of the optimization problem for the GOY model and defined a specific steepest descent numerical approach. Numerical results are also discussed in this section. Then, in section 5, we formulate the optimization problem in an optimal control framework in order to investigate the issues arising in more complex model contexts. A maximum principle of the Pontryagin type is presented and the conditions are discussed having in mind the explicit computation of the solution for two initial conditions. Numerical schemes/strategies using the Maximum Principle for systems with larger dimensions will be discussed in a forthcoming paper.

2 The Obukhov model

Obukhov [Obukhov, 1971] was the first who proposed a shell model having in mind to find a simple nonlinear dynamic system capable of preserving the volume invariance in the phase space. Although structurally similar, this model is not inspired directly from the Navier-Stokes equations. It possesses quadratic nonlinear terms and linear dissipative terms. If one restricts the nonlinear term to nearest-neighbor interactions, then the time evaluation equation is

$$\left(\frac{d}{dt}+\nu k_n^2\right)u_n = a_{n-1}u_{n-1}u_n - a_n u_{n+1}^2 + f_n \quad (1)$$

where a_n's are the nonlinear interaction coefficients, ν is the viscosity, and only f_1 is nonzero, that is,

$$f_n = f\,\delta_{n,1}\,, \quad (2)$$

where δ is a Kronecker symbol. In order for the model to display an energy cascade from large to small scales, the energy must be injected at the large scales (small wave-numbers), flow through an inertial range, and be dissipated at the small scales (large wave-numbers).

3 The Gledzer-Okhitani-Yamada model

The Gledzer model was first proposed as a real-valued model, [Gledzer, 1973]. Later, [Yamada and Ohkitani, 1987] considered its extension to complex-valued model, where they introduced, for given initial conditions,

$$\mathcal{L}\boldsymbol{u} = f_n, \quad (3)$$

being $\mathcal{L}\boldsymbol{u}$ the operator defined by:

$$\mathcal{L}\boldsymbol{u} := \frac{du_n}{dt} - ik_n(u_{n+1}u_{n+2} - \frac{\varepsilon}{q}u_{n-1}u_{n+1} + \frac{\varepsilon-1}{q^2}u_{n-2}u_{n-1})^* + \nu k_n^2 u_n.$$

Here, the superscript $*$ denotes the complex conjugation, ν is the kinematic viscosity, ε is the 2D/3D selector (3D, for $\varepsilon = 1/2$), f_n the external force applied to the n^{th} shell, and $k_n = k_0 q^n$, being ε and q free parameters.

In [Pisarenko *et al.*, 1993], this model was nicknamed the GOY (Gledzer-Okhitani-Yamada) model. The reader can find in these references the connection and the interest of this model associated to the theory of the dynamic systems, as well as to the theory of the turbulence. For any solution of GOY model, we define the structure function [Biferale, 2003],

$$S_p(k_n) \equiv \langle |u_n|^p \rangle = C_0 k_n^{\zeta(p)},$$

where $\zeta(p) = p/3$ according to the K41 theory (i.e. without energy-cascade intermittency) and C_0 a nondimensional constant of order of unity [Constantin *et al.*, 1994]. Here, $\langle |u_n|^p \rangle$ is defined as an average over time, i.e.,

$$\langle |u_n|^p \rangle = \frac{1}{T}\int_0^T |u_n(t)|^p dt.$$

Long numerical runs (hundreds of millions of time steps), with parameter values $N = 25$, $\nu = 5\times10^{-7}$, $k_0 = 0.05$, and $q = 2$, and with $f_n = 0.1(1+i)\delta_{n,0}$, determine for $\zeta(4)$ and $\zeta(6)$ the following numerical values $\zeta^{\mathrm{NV}}(4) = 1.26(3)$, and $\zeta^{\mathrm{NV}}(6) = 1.76(5)$. Other values for different p's can be found in [Biferale, 2003].

Our goal is to find a forcing, f_n, which results in a solution of the GOY with these scaling exponents, but in a much shorter time interval, say $[0, T]$. With this in mind, consider the following cost functional

$$\mathcal{J}(\boldsymbol{f}) \triangleq \frac{1}{2T}\int_0^T\!\!\int_I w(t,k)\left|S_p(k_n) - S_p^{\mathrm{NV}}(k_n)\right|^2 dkdt,$$

where $I = [n_1\,, n_2]$ $(1 < n_1 < n_2 < N)$ is the inertial range of the shell model. The function $w(t,k)$ is a positive weight function which normalizes the error $\left|S_p(k_n) - S_p^{\mathrm{NV}}(k_n)\right|^2$ to get a uniform error distribution over all wave numbers. We may now formulate the following optimization problem:

$$\min_{f\in\mathcal{U}} \mathcal{J}(f),$$

where $\mathcal{U}$ is a suitable function space with a Hilbert structure. The cost functional $\mathcal{J}$ depends on f through the system of ODE (3).

Our goal is to find a forcing $f_{\mathrm{opt}} \in \mathcal{U}$ that minimizes the cost functional $\mathcal{J}$.

4 Mathematical formulation of an optimization problem for the GOY model

The necessary condition characterizing the minimizer f_{opt} of the cost functional is the vanishing of Gâteaux differential $\mathcal{J}'$, i.e.

$$\mathcal{J}'(f_{opt}, f') = 0,$$

for all $f' \in \mathcal{U}$, where the Gâteaux differential is defined by

$$\mathcal{J}'(f;\, f') \triangleq \lim_{\delta\to0}\frac{\mathcal{J}(f+\delta f') - \mathcal{J}(f)}{\delta},$$

if the limit exists. If this limit does in fact exist for all $f' \in \mathcal{U}$, then $\mathcal{J}$ is Gâteaux differentiable at f. After some calculation, it can be shown that

$$\mathcal{J}'(f; f') = \frac{1}{2T}\int_0^T \sum_{n=1}^{N} w(t,k_n)(S_p(k_n) - S_p^{\mathrm{NV}}(k_n)) \times (u_n u_n'^* + u_n' u_n^*)dt\,,$$

where u'_n is the solution of the GOY model equation linearized around the state u_n , i.e.,

$$\begin{aligned} Lu' := \frac{du'_n}{dt} - ik_n((u_{n+1}u'_{n+2} + u'_{n+1}u_{n+2}) \\ -\frac{\epsilon}{q}(u_{n-1}u'_{n+1} + u'_{n-1}u_{n+1}))^* \\ -i\frac{\epsilon-1}{q^2}k_n(u_{n-1}u'_{n-2} + u'_{n-1}u_{n-2})^* \\ +\nu k_n^2 u'_n = f'_n. \end{aligned}$$

On the other hand, the Riesz representation theorem, [Kolmogorov and Fomin, 1999], guarantees the existence of a unique element $\nabla\mathcal{J}$ which satisfies the identity

$$\mathcal{J}'(f;f') = \langle \nabla\mathcal{J}, f'\rangle.$$

By using a suitably defined adjoint variable $u^\dagger$, we have

$$\langle u^\dagger, f'\rangle = \langle u^\dagger, Lu'\rangle = \langle L^\dagger u^\dagger, u'\rangle,$$

where the adjoint operator $L^\dagger$ is

$$L^\dagger u^\dagger = \begin{bmatrix} w(t,k_1)(S_p(k_1) - S_p^{\mathrm{NV}}(k_1))u_1 \\ w(t,k_2)(S_p(k_2) - S_p^{\mathrm{NV}}(k_2))u_2 \\ w(t,k_3)(S_p(k_3) - S_p^{\mathrm{NV}}(k_3))u_3 \\ \vdots \\ w(t,k_N)(S_p(k_N) - S_p^{\mathrm{NV}}(k_N))u_N \end{bmatrix}$$

Now, consider the following decomposition for the operator L :

$$L\boldsymbol{u}' = \left(\frac{d}{dt} - iAC + \nu B\right)\boldsymbol{u}' ,$$

where

$$\boldsymbol{u}' = \begin{bmatrix} u'_1 \\ u'_2 \\ u'_3 \\ \vdots \\ u'_N \end{bmatrix},$$

the matrix A is such that

$$A^* = \begin{bmatrix} 0 & a_{1,2} & a_{1,3} & 0 & \cdots & 0 & 0 \\ a_{2,1} & 0 & a_{2,3} & a_{2,4} & \cdots & 0 & 0 \\ a_{3,1} & a_{3,2} & 0 & a_{3,4} & \cdots & 0 & 0 \\ 0 & a_{4,2} & a_{4,3} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & a_{N-3,N-1} & 0 \\ 0 & 0 & 0 & 0 & \cdots & a_{N-2,N-1} & a_{N-2,N} \\ 0 & 0 & 0 & 0 & \cdots & 0 & a_{N-1,N} \\ 0 & 0 & 0 & 0 & \cdots & a_{N,N-1} & 0 \end{bmatrix},$$

where the coefficients of the matrix are given by

$$\begin{aligned} & a_{1,2} = k_1(u_3 + bu_0), \quad a_{1,3} = k_1u_2 \\ & a_{2,1} = k_2(bu_3 + cu_0), \quad a_{2,3} = k_2(u_4 + bu_1), \\ & a_{3,1} = ck_3u_2, \quad a_{3,2} = k_3(bu_4 + cu_1), \\ & a_{2,4} = k_2u_3, \quad a_{3,4} = k_3(u_5 + bu_2) \\ & a_{4,2} = ck_4u_3, \quad a_{4,3} = k_4(bu_5 + cu_2) \\ & a_{N-3,N-2} = k_{N-3}(u_{N-1} + bu_{N-4}) \\ & a_{N-2,N-3} = k_{N-2}(bu_{N-1} + cu_{N-4}) \\ & a_{N-2,N} = k_{N-2}u_{N-1}, \quad a_{N-1,N-3} = ck_{N-1}u_{N-2} \\ & a_{N-1,N-2} = k_{N-1}(bu_N + cu_{N-3}) \\ & a_{N-3,N-1} = k_{N-3}u_{N-2} \\ & a_{N-2,N-1} = k_{N-2}(u_N + bu_{N-3}) \\ & a_{N-1,N} = k_{N-1}(u_{N+1} + bu_{N-2}) \end{aligned}$$

with the boundary conditions

$$u_{-1} = u_0 = u_{N+1} = u_{N+2} = 0,$$

and the operator C and B given by

$$C\boldsymbol{u'} = \boldsymbol{u'}^*,$$

(i.e. C is the complex congugate operator)

$$B = \begin{bmatrix} k_1^2 & 0 & 0 & \dots & 0 \\ 0 & k_2^2 & 0 & \dots & 0 \\ 0 & 0 & k_3^2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & k_N^2 \end{bmatrix}.$$

Let us define the operator L in the form

$$L = \frac{d}{dt} + \mathbb{A},$$

where

$$\mathbb{A} = -iAC + \nu B.$$

We have

$$\begin{aligned}\langle f, Lg\rangle &= \int_a^b f(t)(Lg)^* dt \\ &= \int_a^b f(t)\left[\frac{dg^*(t)}{dt} + \mathbb{A}^* g^*(t)\right] dt \\ &= \int_a^b f(t)\frac{dg^*(t)}{dt}dt + \int_a^b f(t)\mathbb{A}^* g^*(t)dt \\ &= -\int_a^b \frac{df(t)}{dt} g^*(t)dt + \int_a^b f(t)\mathbb{A}^* g^*(t)dt \\ &= \int_a^b g^*(t)\left[-\frac{df(t)}{dt} + \mathbb{A}^H f(t)\right] dt \\ &= \left\langle g^*, (-\frac{df(t)}{dt} + \mathbb{A}^H f(t))^* \right\rangle \\ &= \left\langle g, -\frac{df(t)}{dt} + \mathbb{A}^H f(t) \right\rangle^* \\ &= \left\langle -\frac{df(t)}{dt} + \mathbb{A}^H f(t),\, g \right\rangle \\ &= \left\langle \left(-\frac{d}{dt} + \mathbb{A}^H\right) f,\, g \right\rangle,\end{aligned}$$

where $\mathbb{A}^H = \mathbb{A}^{*\dagger}$ and the fact that $[f(t)g^*(t)]_{t=a}^b$ vanishes due to the boundary conditions was used. Then, the Gâteaux derivative can be rewritten as $\mathcal{J}'(f;\, f') = \langle L^\dagger u^\dagger, u'\rangle$. Therefore,

$$\nabla\mathcal{J} = u^\dagger.$$

Hence, the gradient direction $\nabla\mathcal{J}$ can be conveniently expressed in terms of the solution to the following adjoint system:

$$\begin{aligned}L^\dagger u^\dagger &= \left(-\frac{d}{dt} + \mathbb{A}^H\right) u^\dagger \\ &= -\frac{d}{dt}u^\dagger + \mathbb{A}^H u^\dagger \\ &= -\frac{d}{dt}u^\dagger + (-iAC + \nu B)^H u^\dagger \qquad (4) \\ &= \begin{bmatrix} w(t,k_1)\,(S_p(k_1) - S_p^{\mathrm{NV}}(k_1))\,u_1 \\ w(t,k_2)\,(S_p(k_2) - S_p^{\mathrm{NV}}(k_2))\,u_2 \\ w(t,k_3)\,(S_p(k_3) - S_p^{\mathrm{NV}}(k_3))\,u_3 \\ \vdots \\ w(t,k_N)\,(S_p(k_N) - S_p^{\mathrm{NV}}(k_N))\,u_N \end{bmatrix}\end{aligned}$$

4.1 Numerical strategy

By using the results from the previous section, we can now delineate a recursive algorithm that the generates successive updates of the force so that the cost function $\mathcal{J}$ decreases monotonically. Our goal is to find a forcing f_{opt} that minimizes the cost functional $\mathcal{J}$. By starting with an initial guess $f^{(0)}$, an approximation of the minimizer can be founded using a gradient-based descent method of the form

$$f^{(n+1)} = f^{(n)} + \tau^{(n)}\mathcal{A}\nabla\mathcal{J}(f^{(n)}),\ n = 1, 2, \cdots \qquad (5)$$

such that $\lim_{n\to\infty} f^{(n)} = f_{opt}$, where n is the iteration count and $\tau^{(n)} \in \mathbb{R}^-$ is a constant to be determined at each iteration (for instance, by the search line method [Press *et al.*, 2007]). At each iteration, the descent direction $\mathcal{A}\nabla\mathcal{J}$ is computed based on the gradient of cost functional $\nabla\mathcal{J}$.

To summarize, the optimization process can be expressed in the following algorithm.

1. Choose an initial guess $f^{(0)}$; $n = 0$.
2. Solve GOY model equation with $f = f^{(n)}$.
3. Solve adjoint equation (4).
4. Obtain the cost functional gradient as $\nabla\mathcal{J} = u^\dagger$.
5. Find parameter $\tau^{(n)}$ through line minimization.
6. Update the control variable through (5); $n = n+1$.
7. Go back to step 2.

5 Maximum principle for the Obukhov model

In this section, we will consider the Obuhkov model with $N = 3$ shells. Consider the following optimal control problem

$$\begin{aligned}\text{Minimize} \quad & J[x,u] \\ \text{subject to} \quad & \dot{x} = F(x) + u \\ & x(0) = x_0 \\ & u \in [-M, M]\end{aligned}$$

where the cost functional is defined by

$$J[x,u] = \frac{1}{2}\int_0^T [(x_1(t)-1)^2 + (x_2(t)-1)^2 + (x_3(t)-1)^2]\, dt,$$

with

$$F(x) = \begin{bmatrix} 2\rho x_2 x_3 - \lambda x_1 \\ -\rho x_1 x_3 - \lambda x_2 \\ -\rho x_1 x_2 - \lambda x_3 \end{bmatrix},$$

and

$$u = \begin{bmatrix} u_1 \\ 0 \\ 0 \end{bmatrix}.$$

Here, u is a measurable control with

$$u_1 \in [-M, M],$$

being $M > 0$, $x(0)$ is the initial state variable value, and $t \in [0, T]$. The necessary conditions of optimality in the form of a Maximum Principle of Pontryagin, [Pontryagin *et al.*, 1962], will be used in order to characterize the solution to the above optimal control problem.

Let H be the Pontryagin function defined by

$$H(x, p, u) = p^T F(x) + p^T u - \frac{1}{2} \sum_{i=1}^{3} (x_i - 1)^2$$

where $p^T = (p_1, p_2, p_3)$.

By using the maximum condition

$$H(x, p, u^*) = \max_{|u| \leq M} H(x, p, u),$$

we get

$$u^*(t) = (M \operatorname{sign}(p_1(t), 0, 0))^T .$$

The adjoint system is given by

$$-\dot{p}^T = \frac{\partial H}{\partial x} = p^T D_x F(x) - (x - \mathbf{1})^T$$

where we have used the following compact notation

$$x = (x_1, x_2, x_3)^T,$$

$$\mathbf{1}^T = (1, 1, 1),$$

and

$$D_x F(x) = \begin{bmatrix} -\lambda & 2\rho x_3 & 2\rho x_2 \\ -\rho x_3 & -\lambda & -\rho x_1 \\ -\rho x_2 & -\rho x_1 & -\lambda \end{bmatrix}.$$

In order to illustrate the application of the Maximum Principle for this optimal control problem, we solve the two point boundary value problem arising form the Maximum Principle conditions by using the so-called shooting methods for the simple case for which $x_1(0) = x_2(0) = x_3(0) = 0$.

It is obvious that, in this case we have, we have $x_2(t) = x_3(t) = 0$, and the dynamics are reduced to

$$\dot{x}_1(t) = -\lambda x_1(t) + 1,$$

i.e.,

$$x_1(t) = \frac{1}{\lambda} \left(1 - e^{-\lambda t}\right) + x_1^0 e^{-\lambda t}.$$

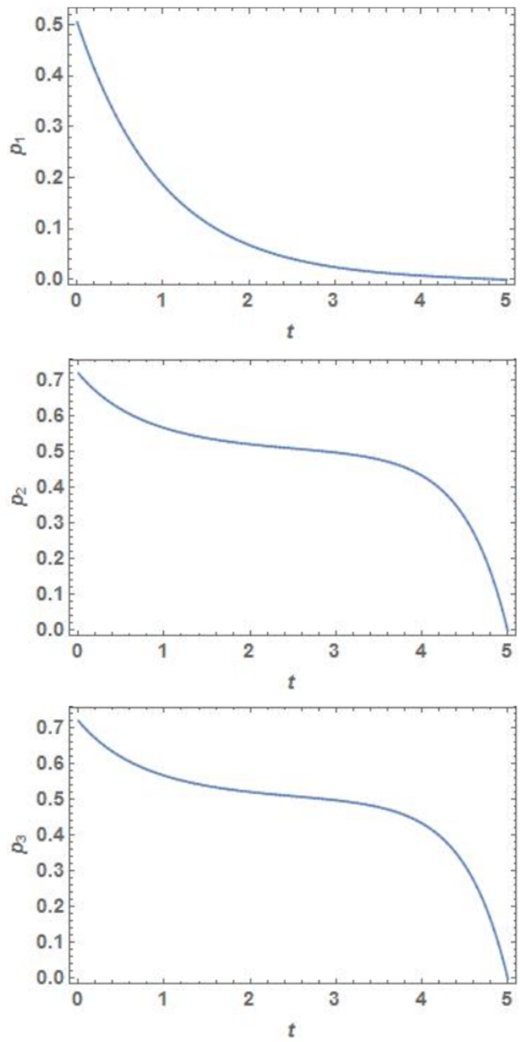

Figure 1. Graphics of the adjoint variables for T = 5.

Thus, the adjoint system becomes

$$\begin{cases} \dot{p}_1(t) = \lambda p_1(t) + \frac{1}{\lambda}\left(1 - e^{-\lambda t}\right) + x_1^0 e^{-\lambda t} - 1\,, \\ \dot{p}_2(t) = \lambda p_2(t) + \rho p_3(t)\left(\frac{1}{\lambda}\left(1 - e^{-\lambda t}\right) + x_1^0 e^{-\lambda t}\right) - 1\,, \\ \dot{p}_3(t) = \rho p_2(t)\left(\frac{1}{\lambda}\left(1 - e^{-\lambda t}\right) + x_1^0 e^{-\lambda t}\right) + \lambda p_3(t) - 1, \end{cases}$$

and we conclude that

$$p_1(t) = e^{-\lambda(T-t)} \left[\frac{e^{-\lambda T}}{2\lambda} \left(x_1^0 - \frac{1}{\lambda} \right) + \frac{(1-\lambda)}{\lambda^2} \right] - \frac{e^{-\lambda T}}{2\lambda} \left(x_1^0 - \frac{1}{\lambda} \right) - \frac{(1-\lambda)}{\lambda^2}.$$

The determination of the adjoint variables $p_2(\cdot)$ and $p_3(\cdot)$ is done by numerical integration, whose result is shown in Figure 1.

6 Conclusion

As a general conclusion, we note that the theoretical results reported here point for the possibility of reducing the computation time so that the systems defined by shell models rapidly attain the steady state regime in the phase space where the structure functions are characterized by power laws.

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