K-41 Optimized Approximate Deconvolution Models

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Abstract: If the Navier-Stokes equations are averaged with a local, spacial convolution type filter, $\overline{\boldsymbol{\phi}} = g_\delta * \boldsymbol{\phi}$, the resulting system is not closed due to the filtered nonlinear term $\overline{\mathbf{uu}}$. An approximate deconvolution operator D is a bounded linear operator which satisfies

$$\mathbf{u} = D(\overline{\mathbf{u}}) + O(\delta^\alpha),$$

where δ is the filter width and $\alpha \geq 2$. Using a deconvolution operator as an approximate filter inverse yields the closure

$$\overline{\mathbf{uu}} = \overline{D(\overline{\mathbf{u}})D(\overline{\mathbf{u}})} + O(\delta^\alpha).$$

We derive optimal approximate deconvolution models for $3D$ turbulence. Specifically, we find the optimal parameters that minimize the time averaged consistency error of approximate deconvolution operators and models for time averaged, fully developed, homogeneous, isotropic turbulence.

We answer important questions of *How to adapt deconvolution procedures to velocities from homogeneous, isotropic turbulent flows?* and *What is the increase in accuracy that results?*

Keywords: Navier-Stokes equations, large eddy simulation, approximate deconvolution model, turbulence

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1 INTRODUCTION

The grand problem of singular perturbations is turbulence: the behavior of the solution of the Navier-Stokes equations (NSE) as the Reynolds number, Re, increases and the NSE reduce to the Euler equation. For many turbulent flows it is known that suitable velocity averages retain regularity as $Re \to \infty$. We show how to exploit this in the design of algorithms for turbulent flow simulation. Various turbulence models are used for simulations seeking to predict flow statistics or averages. In large eddy simulation (LES) the evolution of local, spacial averages is sought. The accuracy of a model measured in a chosen norm, $||\cdot||$, i.e.

$$||\textit{averaged NSE solution} - \textit{LES solution}||,$$

can be assessed in several experimental and analytical ways. One important analytical approach is to study the model's *consistency error* as a function of the averaging radius δ and the Reynolds number Re.

This report studies the model's *consistency error* of approximate deconvolution models as begun in [LL06]. Our goal is to minimize the time averaged consistency error of approximate deconvolution models (ADM) for fully developed, homogeneous, isotropic turbulence.

The family of models we consider is based upon the *van Cittert* approximate deconvolution algorithm. Acceleration/relaxation parameters can be introduced at no extra computational cost. This leads to a new approximate deconvolution algorithm, the *Accelerated van Cittert* and a new model for $\overline{\mathbf{u}}$ and $\overline{p}$. We consider the problem of how to select and adapt the parameters to turbulence. Such analytical guidance on parameter selection is inherently interesting; it also helps answer two important questions of *How to adapt deconvolution procedures to data from turbulent velocities?* and *What is the increase in accuracy that results?* Our approach is a direct calculation of the optimal parameters for the iteration applied to functions with the power/energy spectrum $E(k) \sim \alpha\varepsilon^{2/3}k^{-5/3}$ of homogeneous, isotropic turbulence. Using the $K-41$ theory of turbulence, we find optimal parameter values and give a numerical comparison of the models corresponding to the van Cittert and Accelerated van Cittert algorithms.

Let the velocity $\mathbf{u}(x,t)=u_j(x_1,x_2,x_3,t)$, (j=1,2,3) and pressure $p(x,t)=p(x_1,x_2,x_3,t)$ be solutions of the underlying Navier Stokes equations:

$$\begin{aligned} \mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u} - \nu\triangle\mathbf{u} + \nabla p &= \mathbf{f} \text{ in } \mathbb{R}^3 \\ \nabla\cdot\mathbf{u} &= 0 \text{ in } \mathbb{R}^3 \end{aligned} \tag{1.1}$$

where $\nu = \mu/\rho$ is the kinematic viscosity and $\mathbf{f}$ is the body force. We consider the full Cauchy problem to focus on the interior closure model, to separated it from technical problems associated with filtering through a boundary, [DJL], and to postpone the important question of parameter selection inside a turbulent boundary layer, [JLS], until a full treatment of that problem is possible. The results herein are extendable from the Cauchy problem using Fourier transforms (herein) to L-periodic problems using Fourier series. The Navier-Stokes equations are supplemented by the initial condition, the usual pressure normalization condition

$$\mathbf{u}(x,0) = \mathbf{u}_0(x) \text{ and } \int_{\mathbb{R}^3} p dx = 0, \tag{1.2}$$

and the assumption that the solution, its gradient, and all data are square integrable.

Given $\boldsymbol{\phi} \in L^2(\mathbb{R}^3)$, its differentially filtered average, over the selected averaging radius δ, is denoted by $\overline{\boldsymbol{\phi}}$ and is the unique solution of:

$$-\delta^2\triangle\overline{\boldsymbol{\phi}} + \overline{\boldsymbol{\phi}} = \boldsymbol{\phi}. \tag{1.3}$$

Differential filters are well-established in LES, starting with the work of Germano [Ger86] and have many connections to regularization processes such as the Yoshida regularization of semigroups and the work of Foias, Holm, Titi [FHT01] (and others) on Lagrange averaging of the Navier-Stokes equations.

Averaging the NSE shows that the true flow averages satisfy the (non-closed) equations known as the Space Filtered Navier-Stokes Equations (SFNSE)

$$\begin{aligned} \overline{\mathbf{u}}_t + \nabla\cdot(\overline{\mathbf{u}\,\mathbf{u}}) - \nu\triangle\overline{\mathbf{u}} + \nabla\overline{p} &= \overline{\mathbf{f}} \\ \nabla\cdot\overline{\mathbf{u}} &= 0. \end{aligned} \tag{1.4}$$

An approximate deconvolution operator D is a bounded operator, $D : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ satisfying

$$\boldsymbol{\phi} = D\overline{\boldsymbol{\phi}} + O(\delta^\alpha), \text{ for smooth } \boldsymbol{\phi} \text{ and } \alpha \geq 2.$$

In other words, D is an asymptotic (as $\delta \to 0$) approximate inverse of G. Given an approximate deconvolution operator, the closure problem in the SFNSE can be solved approximately (but systematically) by:

$$\overline{\mathbf{u}\,\mathbf{u}} \simeq \overline{D\overline{\mathbf{u}}\ D\overline{\mathbf{u}}} + O(\delta^\alpha),$$

for smooth $\mathbf{u}$ or in smooth flow regions. This closure approximation leads to approximate deconvolution model of turbulence

$$\begin{aligned} \mathbf{w}_t + \nabla\cdot(\overline{D\mathbf{w}\ D\mathbf{w}}) - \nu\triangle\mathbf{w} + \nabla q &= \overline{f} \\ \nabla\cdot\mathbf{w} &= 0. \end{aligned} \tag{1.5}$$

Our estimates are based on assumptions on time averages of solutions of the NSE which are implied for homogeneous, isotropic turbulence by the Kolmogorov $K-41$ theory.

The most important components of the $K-41$ theory are the time (or ensemble) averaged energy dissipation rate, ε, and the distribution of the flow's kinetic energy across wave numbers, $E(k)$. Let $< \cdot >$ denote time averaging

$$< \boldsymbol{\phi} > (x) := \overline{\lim_{T\to\infty}}\frac{1}{T}\int_0^T \boldsymbol{\phi}(x,t)dt. \tag{1.6}$$

Given the velocity field of a particular flow, $\mathbf{u}(x,t)$, the (time averaged) energy dissipation rate of that flow is defined to be:

$$\varepsilon := \overline{\lim_{T\to\infty}}\frac{1}{T}\int_0^T \frac{1}{L^3}\int_{\mathbb{R}^3} \nu|\nabla\mathbf{u}(x,t)|^2 dx\ dt, \tag{1.7}$$

where $|\nabla\mathbf{u}(x,t)|^2 = \frac{\partial u^i}{\partial x_j}(x,t)\cdot\frac{\partial u^i}{\partial x_j}(x,t)$.

The K-41 theory states that at high enough Reynolds numbers there is a range of wave numbers

$$0 < k_{\min} := U\nu^{-1} \leq k \leq \varepsilon^{\frac{1}{4}}\nu^{-\frac{3}{4}} =: k_{\max} < \infty, \tag{1.8}$$

known as the inertial range, beyond which the kinetic energy in $\mathbf{u}$ is negligible, and in this range

$$E(k) \doteq \alpha\varepsilon^{\frac{2}{3}}k^{-\frac{5}{3}}, \tag{1.9}$$

where α (in the range 1.4 to 1.7) is the universal Kolmogorov constant, k is the wave number and ε is the particular flow's energy dissipation rate. The energy dissipation rate ε is the only parameter which differs from one flow to another. Outside the inertial range the kinetic energy in the small scales decays exponentially. Thus, $E(k) \leq \alpha\varepsilon^{\frac{2}{3}}k^{-\frac{5}{3}}$ since $E(k) \simeq 0$ for $k \geq k_{\max}$ and $E(k) \leq E(k_{\min})$ for $k \leq k_{\min}$.

2 Consistency Error of Turbulence Models

In general, suppose $\mathbf{u}$ satisfies $N_{true}(\mathbf{u}) = \mathbf{f}$ and $\mathbf{w}$, an approximation to $\overline{\mathbf{u}}$, satisfies the approximate reduced model

$$N_{Reduced}(\mathbf{w}) = \overline{\mathbf{f}} \tag{2.1}$$

The true equation can be rewritten as $\overline{N_{true}(\mathbf{u})} = \overline{\mathbf{f}}$ or

$$N_{Reduced}(\overline{\mathbf{u}}) = \overline{\mathbf{f}} - \left[N_{Reduced}(\overline{\mathbf{u}}) - \overline{N_{true}(\mathbf{u})}\right] \tag{2.2}$$

Definition 2.1. *The modelling error is* $\mathbf{e} = \overline{\mathbf{u}} - \mathbf{w}$ *while the reduced model's consistency error or residual stress is the residual of* $\overline{\mathbf{u}}$ *in the approximate reduced model:*

$$\boldsymbol{\tau}(\mathbf{u}) = \overline{N_{true}(\mathbf{u})} - N_{Reduced}(\overline{\mathbf{u}}). \tag{2.3}$$

Comparing (2.2) to (2.1), the *deviation* of $\overline{\mathbf{u}}$ from $\mathbf{w}$ is driven by the consistency error $\boldsymbol{\tau}(\mathbf{u})$. If an appropriate setting is selected for (2.1) and (2.2) under which the operators involved are C^1, the error $\mathbf{e} = \overline{\mathbf{u}} - \mathbf{w}$ satisfies

$$\int_0^1 N'_{Reduced}(s\overline{\mathbf{u}} + (1-s)\mathbf{w})\mathbf{e}\; ds = \boldsymbol{\tau}(\mathbf{u}).$$

The error is thus driven by the turbulence model's consistency error and the error's size is related to the stability properties of the linearization of the reduced model. From either point of view, a small modelling error depends on a reduced model with

(i) small consistency error, and

(ii)a sufficiently stable linearization.

When this framework is specialized to LES models of turbulence, the consistency error is often called the *residual stress*, [LL06], and is derived next.

Example 1. Given an approximate deconvolution operator and the associated ADM, the model's error $\overline{\mathbf{u}} - \mathbf{w}$ is driven by the error in the deconvolution process itself. Indeed, the exact SFNSE can be rewritten as:

$$\overline{\mathbf{u}}_t + \nabla \cdot (\overline{D\overline{\mathbf{u}}\; D\overline{\mathbf{u}}}) - \nu\triangle\overline{\mathbf{u}} + \nabla\overline{p} = \overline{\mathbf{f}} + \overline{\nabla \cdot \boldsymbol{\tau}}. \tag{2.4}$$

Definition 2.2. *The error in the model (1.5) is* $\mathbf{e} = \overline{\mathbf{u}} - \mathbf{w}$. *The consistency error of the model* (1.5)*,* $\boldsymbol{\tau}(\mathbf{u})$ *and the deconvolution error,* $\mathbf{e}^{DCV}(\mathbf{u})$*, are defined as:*

$$\boldsymbol{\tau}(\mathbf{u}) = D\overline{\mathbf{u}}\; D\overline{\mathbf{u}} - \mathbf{u}\;\mathbf{u},$$

$$\mathbf{e}^{DCV}(\mathbf{u}) = \mathbf{u} - D\overline{\mathbf{u}}.$$

Comparing the exact SFNSE (2.4) to the LES model (1.7), exactly as in (2.1) to (2.3), the model's consistency error $\boldsymbol{\tau}$ drives the deviation of the true flow averages from the model's solution. Further, the model's error, $\mathbf{e} = \overline{\mathbf{u}} - \mathbf{w}$ satisfies

$$\mathbf{e}_t + \nabla \cdot \left(\overline{D\overline{\mathbf{u}}\; D\mathbf{e}} + \overline{D\mathbf{e}\; D\mathbf{w}}\right) - \nu\triangle\mathbf{e} + \nabla(\overline{p} - q) = \overline{\nabla \cdot \boldsymbol{\tau}}, \tag{2.5}$$

which gives a direct link between $\mathbf{e}$ and $\boldsymbol{\tau}$. Consider therefore $\boldsymbol{\tau}$. By rearrangement, $\boldsymbol{\tau}$ satisfies

$$\begin{aligned}\boldsymbol{\tau} &= D\overline{\mathbf{u}}\;(D\overline{\mathbf{u}} - \mathbf{u}) + (D\overline{\mathbf{u}} - \mathbf{u})\;\mathbf{u}\\ &= D\overline{\mathbf{u}}\mathbf{e}^{DCV}(\mathbf{u}) - \mathbf{e}^{DCV}(\mathbf{u})\mathbf{u}.\end{aligned} \tag{2.6}$$

Thus, by (2.5) minimizing the error in an LES-ADM depends on minimizing the model's consistency error $\boldsymbol{\tau}(\mathbf{u})$. By (2.6), minimizing a model's consistency error hinges upon minimizing the deconvolution error $\mathbf{e}^{DCV}(\mathbf{u}) = \mathbf{u} - D\overline{\mathbf{u}}$.

One way to do this is to introduce and choose the relaxation parameters appropriately.

The theoretical results derived in Sections 3 and 4, can be applied to other LES models as well. Examples include the following:

Example 2. *Time Relaxation Regularization* [LN06]: This model was introduced by Stolz, Adams and Kleiser and complete mathematical theory was developed by Layton and Neda.

$$\mathbf{w}_t + \mathbf{w} \cdot \nabla\mathbf{w} - \nu\Delta\mathbf{w} + \nabla q + \chi\,(\mathbf{w} - D\overline{\mathbf{w}}) = \overline{\mathbf{f}}.$$

The time relaxation term $\chi\,(\mathbf{w} - D\overline{\mathbf{w}})$ is included to damp strongly the temporal growth of the fluctuating component of $\mathbf{w}$ driven by noise, numerical errors, inexact boundary conditions and so on.

The consistency error of time relaxation regularization model is

$$\boldsymbol{\tau}(\mathbf{u}) = \chi\,(\mathbf{u} - D\overline{\mathbf{u}}) = \chi\mathbf{e}^{DCV}(\mathbf{u}).$$

Example 3. *Leray Deconvolution Model* :

$$\mathbf{w}_t + D\overline{\mathbf{w}} \cdot \nabla\mathbf{w} - \nu\Delta\mathbf{w} + \nabla q = \overline{\mathbf{f}}.$$

The consistency error of the Leray deconvolution model is

$$\boldsymbol{\tau}(\mathbf{u}) = \mathbf{u}\mathbf{u} - D\overline{\mathbf{u}}\mathbf{u} = \mathbf{e}^{DCV}(\mathbf{u})\mathbf{u}.$$

3 Approximate Deconvolution Methods

The basic problem in deconvolution is: *given* $\overline{\mathbf{u}}$ *find* $\mathbf{u}$. In other words, solve the equation:

$$G\mathbf{u} = \overline{\mathbf{u}},\ \text{solve for } \mathbf{u}. \tag{3.1}$$

If the averaging operator is smoothing, the deconvolution problem will not be stably invertible.

Definition 3.1. *An approximate deconvolution operator, $D : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ is an approximate inverse of G satisfying:*

(i) $D : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ is a bounded linear operator and

(ii) $D\overline{\boldsymbol{\phi}} = \boldsymbol{\phi} + O(\delta^\alpha)$, for some $\alpha \geq 2$ and sufficiently smooth $\boldsymbol{\phi}$.

This section considers the van Cittert approximate deconvolution algorithm, [BB98]. The approximation $D_N\mathbf{u}$ is computed by N steps of first order Richardson iteration for the operator equation (3.1).

Algorithm 3.1. [*The van Cittert Algorithm*]:
Choose $\mathbf{u}_0 = \overline{\mathbf{u}}$. For $n = 0, 1, 2, ..., N-1$ perform

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \{\overline{\mathbf{u}} - G\mathbf{u}_n\}.$$

Set $D_N(\overline{\mathbf{u}}) := \mathbf{u}_N$.

For example, the induced closure models corresponding to $N = 0$ and 1 are

$D_0\overline{\mathbf{u}} = \overline{\mathbf{u}}$, *so* $\overline{\mathbf{u}\,\mathbf{u}} \simeq \overline{\overline{\mathbf{u}}\,\overline{\mathbf{u}}} + O(\delta^2)$,

$D_1\overline{\mathbf{u}} = 2\overline{\mathbf{u}} - \overline{\overline{\mathbf{u}}}$, *so* $\overline{\mathbf{u}\,\mathbf{u}} \simeq \overline{(2\overline{\mathbf{u}} - \overline{\overline{\mathbf{u}}})\ (2\overline{\mathbf{u}} - \overline{\overline{\mathbf{u}}})} + O(\delta^4)$.

Since the deconvolution problem is ill posed, convergence of $D_N(\overline{\mathbf{u}})$ to $\mathbf{u}$ as $N \to \infty$ is not expected.

For LES, convergence of the van Cittert approximation $D_N\overline{\mathbf{u}}$ to $\mathbf{u}$ as $N \to \infty$ (the classical question for iterations) is not as significant as convergence of $D_N\overline{\mathbf{u}}$ to $\mathbf{u}$ as $\delta \to 0$ and the asymptotic order of accuracy as $\delta \to 0$ for fixed N. When the averaging is given by a differential filter, the accuracy of $D_N\overline{\mathbf{u}}$ as an approximation to $\mathbf{u}$ for smooth functions was addressed by Stolz and Adams [AS01], Berselli, Iliescu and Layton [BIL04], and Dunca and Epshteyn [DE06], in the following.

Lemma 3.1. *Let the averaging operator be given by the differential filter $G\boldsymbol{\phi} := (-\delta^2\triangle + 1)^{-1}\boldsymbol{\phi}$. For any $\boldsymbol{\phi} \in L^2(\mathbb{R}^3)$,*

$$\begin{aligned}\boldsymbol{\phi} - D_N\overline{\boldsymbol{\phi}} &= \left[I - (-\delta^2\triangle + 1)^{-1}\right]^{N+1}\boldsymbol{\phi}\\ &= (-1)^{N+1}\delta^{2N+2}\triangle^{N+1}\overline{\boldsymbol{\phi}}\quad .\end{aligned}$$

Proof. See [AS01] and [DE06]. □

In [LL06], the time averaged error in the van Cittert deconvolution procedure was estimated.

Theorem 3.1. *Under the $K - 41$ theory*

$$< ||\mathbf{u} - D_N\overline{\mathbf{u}}||^2_{L^2(\mathbb{R}^3)} > \leq \left(\frac{3}{2} + \frac{1}{4N + \frac{10}{3}}\right)\alpha C_1^{\frac{2}{3}} U^2 L^3 \left(\frac{\delta}{L}\right)^{\frac{2}{3}}.$$

Proof. The proof follows from [$LL06$]. □

Remark 3.1. *Much theory on filtering is developed in terms of transfer function or symbol of the filtering operator under Fourier transform. Consider the differential filter given by (1.3). The Fourier transform of (1.3) is*

$$\left[\delta^2(k_1^2 + k_2^2 + k_3^2)^2 + 1\right]\widehat{\overline{\phi}}(\boldsymbol{k}) = \widehat{\phi}(\boldsymbol{k}), \qquad (3.2)$$

where $\boldsymbol{k} = (k_1, k_2, k_3)$ is the dual variable of the Fourier transform. Denote by $k = |\boldsymbol{k}| = \sqrt{k_1^2 + k_2^2 + k_3^2}$ the magnitude of $\boldsymbol{k}$. Then (3.2) gives

$$\frac{1}{\delta^2|\boldsymbol{k}|^2 + 1}\widehat{\phi}(\boldsymbol{k}) = \widehat{\overline{\phi}}(\boldsymbol{k}) \qquad (3.3)$$

and thus the transfer function or symbol of the filter is:

$$\widehat{G}(k) = \frac{1}{\delta^2 k^2 + 1}. \qquad (3.4)$$

Relaxation parameters can be introduced into Algorithm 3.1 without any increase in computational effort.

Algorithm 3.2. [*Accelerated van Cittert Algorithm*]:
Given relaxation parameters ω_n, choose $\mathbf{u}_0 = \overline{\mathbf{u}}$. For $n = 0, 1, 2, ..., N-1$ perform

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \omega_n\{\overline{\mathbf{u}} - G\mathbf{u}_n\}.$$

Set $D_N^\omega\overline{\mathbf{u}} := \mathbf{u}_N$.

Further, a recursion formula for D_N^ω can be proven.

Lemma 3.2. *For $N = 0, 1, 2, ...$ the following holds true*

$$D_{N+1}^\omega = D_N^\omega + \omega_N(I - D_N^\omega G).$$

Proof. Indeed, note that $D_0^\omega = I$, where I is the identity operator on $L^2(\mathbb{R}^3)$. Further more, for any integer $N > 1$

$$\begin{aligned}D_{N+1}^\omega\overline{\mathbf{u}} = \mathbf{u}_N + \omega_N\{\overline{\mathbf{u}} - G\mathbf{u}_N\} &= D_N^\omega\overline{\mathbf{u}} + \omega_N\{\overline{\mathbf{u}} - GD_N^\omega\overline{\mathbf{u}}\}\\ = (D_N^\omega + \omega_N\{I - D_N^\omega G\})\overline{\mathbf{u}}\ .\end{aligned}$$

Thus, $D_{N+1}^\omega = D_N^\omega + \omega_N(I - D_N^\omega G)$ for every nonnegative integer N. □

The induced closure model corresponding to $N = 1$ is:

$$D_1^\omega\overline{\mathbf{u}} = (1 + \omega_0)\overline{\mathbf{u}} + \omega_0\overline{\overline{\mathbf{u}}},\ \text{so}$$
$$\overline{\mathbf{u}\,\mathbf{u}} \simeq \overline{((1 + \omega_0)\overline{\mathbf{u}} + \omega_0\overline{\overline{\mathbf{u}}})\ ((1 + \omega_0)\overline{\mathbf{u}} + \omega_0\overline{\overline{\mathbf{u}}})} + O(\delta^4).$$

Next, we analyze in more detail proprieties of the *Accelerated van Cittert* deconvolution operator, D_N^ω.

Lemma 3.3. *Let the averaging operator be the differential filter $G\boldsymbol{\phi} := (-\delta^2\triangle + I)^{-1}\boldsymbol{\phi}$. If the relaxation parameters ω_i are positive, for $i = 0, 1, ..., N$, then the Accelerated van Cittert deconvolution operator $D_N^\omega : \mathrm{L}^2(\mathbb{R}^3) \to \mathrm{L}^2(\mathbb{R}^3)$ is self-adjoint and positive definite.*

Proof. First note that the operator G is bounded, compact and self adjoint. Indeed, multiplying (1.3) by $\overline{\boldsymbol{\phi}}$ and integrating over $\mathbb{R}^3$ leads to

$$0 \leq ||G\boldsymbol{\phi}||^2 \leq ||\boldsymbol{\phi}||^2.$$

This shows that G is bounded and $||G|| \leq 1$. To show G is self-adjoint and positive definite note that for every $\boldsymbol{\phi} \in \mathrm{L}^2(\mathbb{R}^3)$

$$0 \leq \delta^2||\nabla\overline{\boldsymbol{\phi}}||^2 + ||\overline{\boldsymbol{\phi}}||^2 = (\boldsymbol{\phi}, \overline{\boldsymbol{\phi}}) = (\boldsymbol{\phi}, G\boldsymbol{\phi}).$$

We remark that both D_0^ω and D_1^ω are symmetric, as linear combinations of I and G, the identity and the deconvolution operators respectively. Proceeding by induction assume D_l^ω is symmetric. From Lemma 3.2

$$D_{l+1}^\omega = D_l^\omega + \omega_l(I - D_l^\omega G),$$

for every nonnegative integer l. Thus D_{l+1}^ω is symmetric as linear combination of two symmetric operators I and D_l^ω.

Moreover, as in Remark 3.1, the symbol of G satisfies

$$0 < \widehat{G}(k) = \frac{1}{\delta^2 k^2 + 1} \leq 1.$$

Also the symbol of D_1^ω satisfies

$$1 \leq \widehat{D_1^\omega}(k) = 1 + \omega_0 \left(\frac{\delta^2 k^2}{\delta^2 k^2 + 1} \right) \leq 1 + \omega_0$$

for $\omega_0 \geq 0$ by the Spectral Mapping Theorem.

We now prove that the eigenvalues of D_{l+1}^ω are positive between 1 and $1 + \sum_{j=0}^{l} \omega_l$. Proceeding by induction, assume that the eigenvalues of D_l^ω are between 1 and $1 + \sum_{j=0}^{l-1} \omega_l$. Lemma 3.2 and Spectral Mapping Theorem give

$$\lambda(D_{l+1}^\omega) = \lambda(D_l^\omega) + \lambda\left(\omega_k(I - D_l^\omega G)\right)$$

where $\lambda(A)$ denotes the eigenvalues of any operator A. Applying the induction hypothesis $\lambda(D_{l+1}^\omega) = 1 + \sum_{j=0}^{l} \omega_l$, when $k \to 0$ and $\lambda(D_{l+1}^\omega) = 1$ as $k \to \infty$. □

4 K-41 Optimized Approximate Deconvolution Models

This section considers the consistency error of the model

$$\mathbf{w}_t + \nabla \cdot (\overline{D_N^\omega \mathbf{w}\ D_N^\omega \mathbf{w}}) - \nu \triangle \mathbf{w} + \nabla q = \overline{\mathbf{f}}$$
$$\nabla \cdot \mathbf{w} = 0,$$

for turbulent velocity fields. We recall that for $N = 0, 1, 2, ..$

$$\begin{aligned} \boldsymbol{\tau}_N &= D_N^\omega \overline{\mathbf{u}} D_N^\omega \overline{\mathbf{u}} - \mathbf{u}\mathbf{u} \\ &= (D_N^\omega \overline{\mathbf{u}} - \mathbf{u}) D_N^\omega \overline{\mathbf{u}} + \mathbf{u}(D_N^\omega \overline{\mathbf{u}} - \mathbf{u}). \end{aligned} \tag{4.1}$$

Using the time averaged Cauchy-Schwarz inequality and stability bounds, following [LL06], we have:

$$\begin{aligned} < ||\boldsymbol{\tau}_N||_{L^1(\mathbb{R}^3)} > &\leq (1 + ||D_N^\omega \overline{\mathbf{u}}||) < ||\mathbf{u}||^2_{L^2(\mathbb{R}^3)} >^{1/2} \\ & < ||\mathbf{u} - D_N^\omega \overline{\mathbf{u}}||^2_{L^2(\mathbb{R}^3)} >^{1/2}. \end{aligned} \tag{4.2}$$

Thus, estimates for the consistency error in $L^1(\mathbb{R}^3)$ follow from estimates of $< ||\mathbf{u} - D_N \overline{\mathbf{u}}||^2_{L^2(\mathbb{R}^3)} >^{1/2}$. Further optimization of the model's consistency error depends on the minimization of the deconvolution algorithm's error in the appropriate sense.

Lemma 4.1. *Let $\mathbf{e}_N^{DCV} = \mathbf{u} - D_N^\omega \overline{\mathbf{u}}$ be the deconvolution error. Then, $\mathbf{e}_N^{DCV}$ satisfies $\mathbf{e}_0^{DCV} = \mathbf{u} - \overline{\mathbf{u}}$ and for all positive integers N*

$$\mathbf{e}_N^{DCV} = \prod_{i=0}^{N-1} (I - \omega_i G) \mathbf{e}_0^{DCV}. \tag{4.3}$$

Proof. We will use mathematical induction. Note that the conclusion holds true for $N = 1$:

$$\mathbf{e}_1^{DCV} = (I - \omega_0 G)\mathbf{u} - (I - \omega_0 G)\overline{\mathbf{u}} = (I - \omega_0 G)\mathbf{e}_0^{DCV},$$

since $\overline{\mathbf{u}} = G\mathbf{u}$. Assuming $\mathbf{e}_k^{DCV} = \prod_{j=0}^{k-1}(I - \omega_j G)\mathbf{e}_0^{DCV}$ for any k, let us prove

$$\mathbf{e}_{k+1}^{DCV} = \prod_{j=0}^{k} (I - \omega_j G)\mathbf{e}_0^{DCV}.$$

Indeed, since $\mathbf{e}_{k+1}^{DCV}$ can be rewritten as $\mathbf{e}_{k+1}^{DCV} = (I - \omega_k)G\mathbf{u} - (I - \omega_k G)\mathbf{u}_k$ and applying the induction hypothesis we obtain that:

$$\mathbf{e}_{k+1}^{DCV} = \prod_{i=0}^{k} (I - \omega_i G)\mathbf{e}_0^{DCV}, \text{ for all } k \geq 1. \tag{4.4}$$

and therefore (4.3) holds true. □

Lemma 4.2. *We have:*

$$< ||\mathbf{e}_N^{DCV}||^2_{L^2(\mathbb{R}^3)} >=$$
$$\int_{k_{min}}^{k_{max}} \left[\prod_{i=0}^{N-1} (1 - \omega_i \widehat{G}(k)) \right]^2 (1 - \widehat{G}(k))^2 E(k) dk.$$

Proof. Let H_N denote the symbol of $I - D_N^\omega G$. Thus

$$H_N(k) = \left[\prod_{i=0}^{N-1} (1 - \omega_i \widehat{G}(k)) \right]^2 (1 - \widehat{G}(k))^2.$$

Using Parceval's theorem:

$$\begin{aligned} &< ||\mathbf{e}_N^{DCV}||^2_{L^2(\mathbb{R}^3)} >=< ||\hat{\mathbf{e}}_N^{DCV}||^2_{L^2(\mathbb{R}^3)} > \\ &= \overline{\lim_{T->\infty}} \frac{1}{T} \int_0^T \int_{k_{min}}^{k_{max}} H_N(k) |\hat{\mathbf{u}}_N(k,t)|^2 dk \\ &= 2 \int_{k_{min}}^{k_{max}} H_N(k) < \frac{1}{2} |\hat{\mathbf{u}}_N(k,t)|^2 > dk. \end{aligned}$$

But, $E(k) = \int_{k_{min}}^{k_{max}} < \frac{1}{2}|\hat{\mathbf{u}}_N(k,t)|^2 > dk$ and thus

$$< ||\mathbf{e}_N^{DCV}||^2_{L^2(\mathbb{R}^3)} >= 2 \int_{k_{min}}^{k_{max}} H_N(k) E(k) dk,$$

which concludes our proof. □

So, the optimization problem reduces to finding the minimum of the function $F_N : \mathbb{R}_+^N \to \mathbb{R}_+$, where $F_N(\omega_0, ..., \omega_N)$ is:

$$\int_{k_{min}}^{k_{max}} \left[\prod_{i=0}^{N-1} (1 - \omega_i \widehat{G}(k)) \right]^2 (1 - \widehat{G}(k))^2 E(k) dk. \quad (4.5)$$

In the case of fully developed, homogeneous, isotropic turbulence, the integral (4.5) behaves differently for low and high wave numbers. The transition point is the cutoff wave number δ. This leads to several problems for selection of the optimal ω_i. The first problem is find ω_i to minimize

$$\int_{k_{min}}^{k_{max}} \left[\prod_{i=0}^{N-1} (1 - \omega_i \widehat{G}(k)) \right]^2 (1 - \widehat{G}(k))^2 E(k)$$
$$\text{subject to } E(k) = \alpha \varepsilon^{2/3} k^{-5/3}. \quad (4.6)$$

The difficulty with this problem is that the formula used for $E(k)$ only holds on the inertial range and only the resolved scales of that inertial range are calculated. Thus, it is sensible to restrict the scales in (4.6) to the resolved scales of the inertial range. So, we can restrict the problem to finding ω_i to minimize

$$\int_{0}^{\frac{\pi}{\delta}} \left[\prod_{i=0}^{N-1} (1 - \omega_i \widehat{G}(k)) \right]^2 (1 - \widehat{G}(k))^2 E(k)$$
$$\text{subject to } E(k) = \alpha \varepsilon^{2/3} k^{-5/3}. \quad (4.7)$$

We minimize F_N in $\mathbb{R}^N$ by solving the $N \times N$ system:

$$\left(\frac{\partial F_N}{\partial \omega_0}, ..., \frac{\partial F_N}{\partial \omega_{N-1}} \right) = 0. \quad (4.8)$$

We solved the above system for $N = 1, ..., 5$. The $K - 41$ optimized relaxation parameters are given in $Table$ 1.

N	ω_0	ω_1	ω_2	ω_3	ω_4
1	2.10	-	-	-	-
2	2.02	2.02	-	-	-
3	1.44	4.91	1.44	-	-
4	1.49	1.49	5.83	1.49	-
5	1.53	1.53	6.52	1.53	1.53

Table 1: Direct optimized parameters

$Table$ 2 contains estimates of

$$\frac{< \|\widehat{\mathbf{e}}_N^{DCV}\|^2_{L^2(\mathbb{R}^3)} >}{\alpha \varepsilon^{2/3} \delta^{2/3}},$$

when $N = 1, 2, 3, 4, 5$ in the case when the specified parameters are used. It shows the exact improvements in the deconvolution error of the models (1.5), van Cittert versus Accelerated van Cittert for homogeneous, isotropic turbulence, i.e. under the $K - 41$ theory. The van Cittert deconvolution operator corresponds to the case when the relaxation parameters ω_i are all 1. In the calculations we used the and $K - 41$ direct optimized parameters from $Table$ 1.

The reduction in the model's consistency error depends on the order of deconvolution. The Accelerated van Cittert algorithm leads to a model with a consistency error much more smaller than the regular van Cittert.

N	optimized ω_i	unoptimized ω_i
1	0.150	0.258
2	0.068	0.155
3	0.017	0.101
4	0.007	0.070
5	0.003	0.049

Table 2: Normalized Deconvolution Error

5 A Numerical Illustration and Conclusions

For an LES with deconvolution model to be feasible the model's consistency error must be small:

$$< \|\boldsymbol{\tau}\| ><< 1.$$

Thus selection of parameters to minimize model consistency error increases the problems for which LES is feasible and reduces the computational effort of LES.

It is important to note that the use of optimal parameters requires no extra computational effort. Two main results of this work are

(i) the values of those optimal parameters (in section 4) and

(ii) the relative reduction in the model consistency error that results in their use:

$$\frac{\min_{\omega_0,\omega_1,\cdots,\omega_{N-1}} F_N(\omega_0, \omega_1, \cdots, \omega_{N-1})}{F_N(1, 1, \cdots, 1)}$$

is at least 50%. $Table$ 2 reflects the changes in the deconvolution error of the two models we considered. It is important to note that the relative increase in accuracy obtained using optimal parameters itself increases with the order of the model.

The Accelerated van Cittert deconvolution operator is appropriate for many other LES models. We give a numerical example; we consider the Time Relaxation Regularization:

$$\mathbf{w}_t + \mathbf{w} \cdot \nabla \mathbf{w} - \nu \Delta \mathbf{w} + \nabla q + \chi \left(I - D_N G \right)^2 \mathbf{w} = \overline{\mathbf{f}}$$
$$\nabla \cdot \mathbf{w} = 0. \quad (5.1)$$

In (5.1), we study an underresolved flow with recirculation, the flow across a step with $N = 1$. It is known that a particularity of this flow is a recirculating vortex behind the step, which detaches between $Re = 500$ and $Re = 700$. The parabolic inflow profile is given by $\mathbf{u} = (u_1, u_2)^T$, with $u_1 = y(10-y)/25$ and $u_2 = 0$, no-slip boundary conditions are imposed on the top and bottom boundaries, and the "do nothing" boundary condition is used for the outflow.

The computations were performed with the software FreeFem++, see [FF]. The models were discretize in time with the implicit second order Crack-Nicholson scheme and in space order and with the Taylor Hood finite element method, i.e. the velocity was approximated by continuous picewise quadratics and the pressure by continuous picewise linears. The goal of this test is to use the Accelerated van Cittert deconvolution operator in (5.1). The results should be consistent with the well known behavior of the fluid. Behind the step the flow simulation using the optimal parameters corectly develops vortices separate from the step. Figures 1 through 4 show the results at $T = 10, 20, 30, 40$ for $Re = 500$, $\chi = 0.001$, $dt = 0.005$, $\delta = 1.5$.

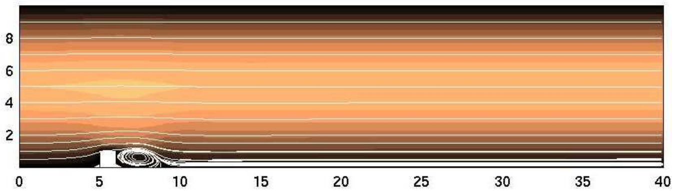

Figure 1: Flow Field at T=10.

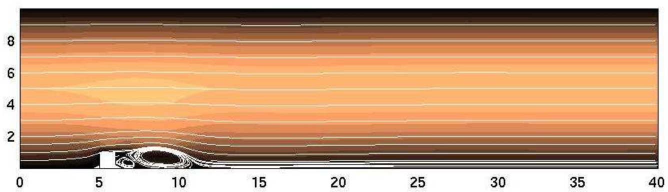

Figure 2: Flow Field at T=20.

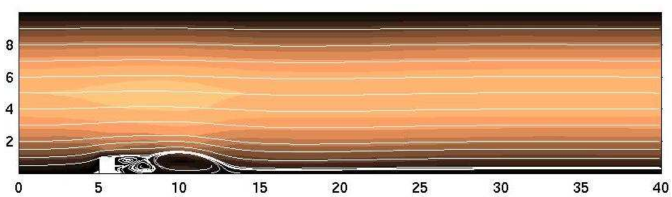

Figure 3: Flow Field at T=30.

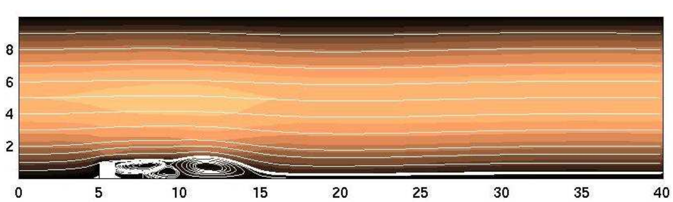

Figure 4: Flow Field at T=40.

The overall analytic conclusion is that higher order models are preferable to lower order models up to the point where their computational cost become prohibitive.

This observation, while surprising from the point of view of traditional error analysis, is consistent with the extensive experiments in the work of Stolz and Adams with the models. We expect that the use of optimized LES-ADMs will only increase further the competitive advantage of higher order models over lower order models.

REFERENCES

[AS01] N. A. Adams and S. Stolz, *Deconvolution methods for subgrid-scale approximation in large eddy simulation*, Modern Simulation Strategies for Turbulent Flow, R.T. Edwards, 2001.

[BB98] M. Bertero and B. Boccacci, *Introduction to Inverse Problems in Imaging*, IOP Publishing Ltd.,1998.

[BIL04] L.C Berselli, T. Iliescu, W. Layton, *Large Eddy Simulation*, Springer, Berlin, 2004

[CD92] P. Constantin and C. Doering, *Energy dissipation in shear driven turbulence*, Phys. Rev. Letters, 69(1992) 1648-1651.

[DJL] A. Dunca, V.John, W. Layton *Approximating local averages of fluid velocities: the equilibrium Navier-Stokes equations* Applied Numerical Mathematics, Volume 49, 2002.

[DE06] A. Dunca and Y. Epshteyn, *On the Stolz-Adams de-convolution LES model*, SIAM J. Math. Anal., 2006, 1890-1902.

[F97] C. Foias, *What do the Navier-Stokes equations tell us about turbulence?* Contemporary Mathematics, 208(1997), 151-180.

[FHT01] C. Foias, D. D. Holm and E. S. Titi, *The Navier-Stokes-alpha model of fluid turbulence*, Physica D, 152-153(2001), 505-519.

[F95] U. Frisch, *Turbulence*, Cambridge, 1995.

[FF] F. Hecht and O. Pironneau , *FreeFem++*, webpage: http://www.freefem.org.

[Ger86] M. Germano, *Differential filters of elliptic type*, Phys. Fluids, 29(1986), 1757-1758.

[JLS] V. John, W. Layton, and N. Sahin, *Derivation and Analysis of Near Wall Models for Channel and Recirculating Flows*, Computers and Mathematics with Applications 48 (2004) 1135-1151.

[LL06] W. Layton and R. Lewandowski, *Residual stress of approximate deconvolution models of turbulence*, Journal of Turbulence vol. 7, 2006, 1-21.

[LN06] W. Layton and M. Neda, *Truncation of scales by time relaxation*, JMAA 325, 2006, 788-807.