1

Towards fluid equations by approximate deconvolution models

Luigi C. Berselli
Dipartimento di Matematica Applicata "U. Dini"
Università di Pisa, Via F. Buonarroti 1/c, Pisa. Italy.
berselli@dma.unipi.it

Abstract We review a selection of recent results linking *approximate deconvolution* operators with the rigorous approximation of the Navier–Stokes equations and their averages.

1.1 Introduction

When studying existence, uniqueness, and other analytical properties of solutions to partial differential equations in many different situations one needs, as a general tool, suitable smoothing/approximation operators. These tools are used to construct approximate initial data and/or approximate equations and are needed, for instance, to show existence through approximation by smooth solutions or to make rigorous calculations that will be otherwise just formal (for example in the study of energy equalities). In the case of the incompressible Navier–Stokes equations (NSE)

$$\text{(NSE)} \qquad \mathbf{u}_t + (\mathbf{u}\cdot\nabla)\,\mathbf{u} - \nu\Delta\mathbf{u} + \nabla p = 0, \tag{1.1}$$

with $\nabla\cdot\mathbf{u} = 0$, these tools have been used, for instance, in the classical paper by Leray (1934), where the convective term $(\mathbf{u}\cdot\nabla)\,\mathbf{u}$ is approximated by $(\rho_\epsilon * \mathbf{u}\cdot\nabla)\,\mathbf{u}$, with $\{\rho_\epsilon\}_{\epsilon>0}$ a classical family of Friedrichs mollifiers. Other applications of smoothing techniques occur also in the study of singular limits, as in Beirão da Veiga (1993) and Majda (1984). See also Kazhikhov (2006), where he studies approximate sequences weakly converging in stronger topologies, with applications to the study of compressible fluids.

Published in *Mathematical Aspects of Fluid Mechanics*, edited by J.C. Robinson, J.L. Rodrigo, & W. Sadowski.

Recently these tools have also been linked with a particular class of Large Eddy Simulation (LES) models and in particular with some aspects of the mathematical theory of *alpha*-models. We recall that LES models provide families of approximate systems which are computationally easier to study than the full NSE, see Sagaut (2001), Geurts (2003), Lesieur, Métais, & Comte (2005), and Berselli, Iliescu, & Layton (2006) for an introduction to some of the aspects of LES. These models, which are designed to be numerical methods for the practical computation of averages of the velocity, are derived by means of different physical, analytical, and numerical insights. In particular, we will review results on approximate deconvolution *alpha*-methods, pointing out that their mathematical analysis has only recently been addressed.

We do not treat any questions about modelling or numerical testing, but we just make a review of some recent results for *high accuracy* models. These models with high accuracy are obtained by introducing approximate deconvolution into some well-known classical models; we will consider them as mathematical methods to produce smooth and stable approximations to the fluid motion, with conserved physical quantities.

We will restrict to the space-periodic case with $\mathbf{x} \in]0, L[^3$ (this is the only setting in which calculations have a sufficient level of mathematical rigour) and we will consider the *differential filter* associated with the Helmholtz operator $A := I - \alpha^2 \Delta$, for some $\alpha > 0$. To this end, given a field $\mathbf{u}$, we define the averaged field $\overline{\boldsymbol{u}}$ as the solution of

$$A\overline{\boldsymbol{u}} = \overline{\boldsymbol{u}} - \alpha^2 \Delta \overline{\boldsymbol{u}} = \mathbf{u},$$

with periodic boundary conditions. It is easy to show that in this setting, if $\nabla \cdot \mathbf{u} = 0$, then $\nabla \cdot \overline{\boldsymbol{u}} = 0$, and $\overline{\boldsymbol{u}}$ is also a solution of the Helmholtz–Stokes system with zero pressure. In the sequel we will denote by $\overline{\ \cdot\ }$ the quantity obtained by application of the *filter*, that is, the inverse of A, i.e. $\overline{\boldsymbol{u}} := A^{-1}\mathbf{u}$. Moreover, if H^s denotes the usual Sobolev space of periodic functions with norm $\|\cdot\|_s$, and $\mathbf{H}^s \subset (H^s)^3$ denotes the subspace of divergence-free fields with zero mean-value, then when $\mathbf{u} \in \mathbf{H}^s$

1. $\overline{\boldsymbol{u}} \in \mathbf{H}^{s+2}$ and $\|\overline{\boldsymbol{u}} - \mathbf{u}\|_{s'} \leq c\,\alpha^{2(s-s')}$ for $s' < s$, and
2. $\overline{\boldsymbol{u}} \to \mathbf{u}$ in $\mathbf{H}^s$, as $\alpha \to 0^+$.

We will apply the ideas of approximate deconvolution to the following three systems (Leray-α, Navier–Stokes-α, and Layton & Lewandowski or simplified Bardina model)

$$\text{(L-}\alpha\text{)} \qquad \mathbf{w}_t + (\overline{\mathbf{w}} \cdot \nabla)\, \mathbf{w} - \nu\Delta\mathbf{w} + \nabla q = 0, \tag{1.2}$$

$$\text{(NS-}\alpha\text{)} \qquad \mathbf{w}_t - \overline{\mathbf{w}} \times (\nabla \times \mathbf{w}) - \nu\Delta\mathbf{w} + \nabla q = 0, \tag{1.3}$$

$$\text{(LL)} \qquad \mathbf{w}_t + \overline{(\mathbf{w} \cdot \nabla)\, \mathbf{w}} - \nu\Delta\mathbf{w} + \nabla q = 0. \tag{1.4}$$

These models are supplemented with $\nabla \cdot \mathbf{w} = 0$, initial datum, and periodic boundary conditions. The external force is set to zero to avoid inessential complications. Here $\mathbf{w}$ denotes a field which is formally closer and closer to the solutions of the NSE as the parameter α becomes smaller and smaller, hence when the averaging defined through A^{-1} approaches the identity I.

Remark 1.1.1 In part of the literature a different notation is used with functions $\mathbf{u}$ and $\mathbf{v}$ such that $\mathbf{v} := \mathbf{u} - \alpha^2\Delta\mathbf{u}$. Up to some changes in the pressure, the three models without deconvolution (1.2), (1.3), and (1.4) are also denoted by

$$\begin{aligned}
&\text{(L-}\alpha\text{)} && \mathbf{v}_t + (\mathbf{u} \cdot \nabla)\, \mathbf{v} - \nu\Delta\mathbf{v} + \nabla q = 0,\\
&\text{(NS-}\alpha\text{)} && \mathbf{v}_t - \mathbf{u} \times (\nabla \times \mathbf{v}) - \nu\Delta\mathbf{v} + \nabla q = 0,\\
&\text{(LL)} && \mathbf{v}_t + (\mathbf{u} \cdot \nabla)\, \mathbf{u} - \nu\Delta\mathbf{v} + \nabla q = 0.
\end{aligned}$$

This notation reflects also a different way in which estimates are written, since they can be stated in terms of $\mathbf{u}$ or of $\mathbf{v}$. Moreover, in several cases the parameter α is replaced by δ, in analogy with the classical notation used in early studies of LES.

We cannot review all the literature concerning these models and we just cite the most theoretical references treating them: therein the interested reader can find further results, related also with numerical computations. The mathematical analysis for the Leray-α model (which is the natural adaptation of Leray's approach in the periodic case) can be found in Cheskidov et al. (2005), while a modified method with regularized convective term $(\mathbf{w} \cdot \nabla)\, \overline{\mathbf{w}}$ has been studied in Ilyin, Lunasin, & Titi (2006). Concerning the NS-α model, also known as the *viscous Camassa–Holm equation*, most of the results are proved in Foias, Holm, & Titi (2002). A modification with nonlinearity given by $-\mathbf{w} \times (\nabla \times \overline{\mathbf{w}})$ and known as NS-ω can be found in Layton et al. (2010). The latter (LL) model is studied in Layton & Lewandowski (2006a). It is also known as the *simplified Bardina* model and has additionally been analysed in Cao, Lunasin, & Titi (2006). Observe too that this model is the same as that of Stolz & Adams when the deconvolution parameter vanishes: see Stolz & Adams, 1999, Stolz, Adams, & Kleiser, 2001, Adams & Stolz, 2001.

These three models have been derived by different approaches: for instance smoothing, clear balance of generalized energies (and models helicity for NS-α without viscosity), and scale similarity, topics which we do not address here. For the interested reader comparison of the conserved quantities can be found in Rebholz (2007); see also Olson & Titi (2007).

The introduction of Approximate Deconvolution Models (ADM) in LES can be understood in the light of the following observation: after having solved one of the above systems, the resulting field $\mathbf{w}$ is smooth, and unique. It also solves a system (formally) close to that solved by $\mathbf{u}$, where $\mathbf{u}$ is a solution of the NSE with the same initial datum. On the other hand, when $\alpha \to 0^+$ it is possible to prove the convergence $\mathbf{w} \to \mathbf{u}$, where $\mathbf{u}$ is a Leray–Hopf weak solution. (This result is proved in the above references and one needs some care to handle this limit rigorously.) Nevertheless, this latter result does not seem to have a terrific impact in applications, since the *radius of the filter* $\alpha > 0$ is related to the mesh size h of the numerical method used to simulate fluid motion. (In our setting this is not the radius, but the name is used by analogy to that related with filtering by convolution with functions of compact support or with Gaussian fields.) The parameter α is related (and it should be of the same order as h) to the smallest persistent scale. Using Fourier series expansions, if $\mathbf{u}(\mathbf{x}) = \sum_{\mathbf{k}\in\mathcal{T}} \mathbf{u}_{\mathbf{k}}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$, with $\mathcal{T} := \frac{2\pi}{L}\mathbb{Z}^3\backslash\{\mathbf{0}\}$, then

$$A^{-1}\mathbf{u} = \sum_{\mathbf{k}\in\mathcal{T}} \frac{\mathbf{u}_{\mathbf{k}}}{1+\alpha^2|\mathbf{k}|^2}\, \mathrm{e}^{\mathrm{i}\,\mathbf{k}\cdot\mathbf{x}}.$$

Consequently, the parameter α is also linked to the amount of damping introduced in high-frequencies. In applications one wishes to solve all relevant scales (full resolution of the flow) and this requires, due to the Kolmogorov K41-theory, that $h = \mathcal{O}(Re^{-3/4})$. For real-life flows this resolution cannot be obtained, due to the constraint of memory capacity of supercomputers currently (and for the foreseeable future) available. This introduces a strong limitation on the values of α which are meaningful when using *alpha*-models in numerical computations.

On the other hand, the overall philosophy behind turbulence modelling is that $\mathbf{w}$ should represent (in a sense to be specified) a "mean velocity". This is reasonable since macroscopic properties are not determined by pointwise behaviour of the velocity or pressure fields, but most likely by their averages. We also expect that, on average, solutions behave in a better way than single trajectories, see Foias et al. (2001b). This poses two serious constraints: the quantity $\mathbf{w}$ needs to be numerically computable and the quantity $\mathbf{w}$ should be close enough to the observable mean fields to be compared with real-life data. This suggests that decreasing α may not be so useful in view of computations. It also challenges us to try to find a way to improve the performance of the method, without dramatically increasing the computational cost. This can be obtained by replacing the filter with another operator that is closer to the identity, but not too expensive to evaluate numerically (in a sense that we will explain later on). Clearly the inversion of the filter (even when invertible!) does not seem to be a good idea, since generally this leads to an ill-conditioned problem. Moreover, the application of the inverse of the filter will have as a result "no-modelling" being introduced in the equations.

A possible implementation of this heuristic idea can be obtained for instance by means of a family of Approximate Deconvolution (AD) operators $\{D_N\}_{N\in\mathbb{N}}$ such that:

1. $D_0 = I$;
2. for each $N \in \mathbb{N}$ the operator D_N is of zero-order (in terms of regularity of Sobolev spaces);
3. *at least formally*

$$D_N \to A, \qquad \text{as } N \to +\infty.$$

Having such a family of operators, the Leray-α model can be replaced by the model with higher accuracy

$$\mathbf{w}_t + (D_N\overline{\mathbf{w}} \cdot \nabla)\,\mathbf{w} - \nu\Delta\mathbf{w} + \nabla q = 0.$$

The convective field $D_N\overline{\mathbf{w}}$ is closer to the field $\mathbf{w}$ than the previous one $D_0\overline{\mathbf{w}} := \overline{\mathbf{w}}$ present in (1.2). Most likely the properties of the model with (AD) are much better than those of Leray-α, which can be seen as a zeroth-order deconvolution model.

In several cases the introduction of a deconvolution operator is suggested, as in Stolz & Adams (1999) with $N \sim 5$, and the practical use in computations is to fix N and α, tuning the parameters to optimize the performance of the code *versus* the numerical instabilities. On the other hand, from the theoretical point of view we would like to have mathematical support for this modelling idea. In order to justify the implementation of deconvolution models, we will study their limiting behaviour, trying to obtain some insight from the analytical results. A review of ADM can also be found in the book by Layton & Rebholz (2012).

Plan of the paper. We will review some of the PDE results concerning the application of AD to the three aforementioned models. In particular, in Section 1.2 we introduce the basics of deconvolution operators and in Section 1.3 we introduce ADM. Next, we will skip all modelling and numerical testing and in Sections 1.4–1.5 we will focus only on the energy spectra and on the rigorous mathematical analysis results which can be obtained by considering the limits $\alpha \to 0^+$ for fixed $N \in \mathbb{N}$, and $N \to +\infty$ for fixed $\alpha > 0$.

1.2 The approximate deconvolution

Once a filter is defined, it is computationally relevant to have an approximate way to invert it. Approximation is needed since, in principle, the filtering operator defined by $G = A^{-1}$ is not invertible, or the inverse is not bounded, or it is not possible to invert it stably, due to a small divisor problem, as with the Gaussian filter (Berselli et al. (2006) §7). For these reasons one wishes to have some kind of a "best approximation for its inversion" or equivalently an approximate solution to the problem: given $\overline{\boldsymbol{u}}$ find $\mathbf{u}$ such that

$$A^{-1}\mathbf{u} = \overline{\boldsymbol{u}}. \tag{1.5}$$

The classical example coming from signal theory is that of a signal filtered by some transmitting/recording device, where the challenge is to reconstruct, in a satisfactory way, the original signal. Early results on deconvolution have been obtained by Wiener (1949), even if the ideas are older and some delay in their diffusion has been caused by the book being classified during World War II. Another field in which one generally uses approximate deconvolution is that of inverse problems as in image reconstruction and, in fact, the first example we will consider comes from this field.

Some deconvolution operators. We review some of the classical deconvolution operators, and we specify them in the case of the Helmholtz operator with periodic boundary conditions, in order to better compare their properties.

van Cittert. The van Cittert (1931) algorithm (common in image reconstruction) is a Richardson iteration for equation (1.5) that works as follows: given $\mathbf{u}_0 := \overline{\boldsymbol{u}}$, set

$$\mathbf{u}_{N+1} := \mathbf{u}_N + (\overline{\boldsymbol{u}} - A^{-1}\mathbf{u}_N).$$

The operator D_N is defined by $D_N\overline{\boldsymbol{u}} := \mathbf{u}_N$. The van Cittert algorithm is based on successive applications of the filter (in fact $\mathbf{u}_1 = 2\overline{\boldsymbol{u}} - \overline{\overline{\boldsymbol{u}}}$, $\mathbf{u}_2 = 3\overline{\boldsymbol{u}} - 3\overline{\overline{\boldsymbol{u}}} + \overline{\overline{\overline{\boldsymbol{u}}}}$, and so on). One of the main properties of this algorithm, in the case of the Helmholtz operators is the following, which is based on a representationb via a truncated von Neumann series, see Dunca & Epshteyn (2006), Stolz et al. (2001), and Berselli et al. (2006) § 8.

Lemma 1.2.1 *Let A^{-1} be defined through the Helmholtz filter. Then, for any $\mathbf{w} \in L^2$ it follows that*

$$\mathbf{w} - D_N\overline{\mathbf{w}} = (-1)^{N+1}\alpha^{2N+2}\Delta^{N+1}A^{-(N+1)}\mathbf{w}.$$

This identity can be used to estimate the residual stress in a precise way for different LES models, see Layton & Lewandowski (2006b). One of the interesting features of the van Cittert operator is that it can be applied also in more complicated situations (boundary value problems) even if its properties are slightly different in that setting (in particular the problem of commutation with first order differential operators arises). By specifying the operator in the periodic setting we can write its symbol as follows: $\widehat{\mathrm{DvC}_N\overline{\boldsymbol{u}}}(\mathbf{k}) := \widehat{\mathrm{DvC}}_{\mathrm{N}}(\mathbf{k})\widehat{\overline{\boldsymbol{u}}}(\mathbf{k})$ with

$$\begin{aligned}\widehat{\mathrm{DvC}}_N(\mathbf{k}) &:= \sum_{n=0}^{N}\left(\frac{\alpha^2k^2}{1+\alpha^2k^2}\right)^n \\ &= (1+\alpha^2k^2)\left[1 - \left(\frac{\alpha^2k^2}{1+\alpha^2k^2}\right)^{N+1}\right],\end{aligned}$$

where $k := |\mathbf{k}|$.

This operator has also an accelerated variant defined by the iteration

$$\mathbf{u}_{N+1} := \mathbf{u}_N + \omega_N(\overline{\boldsymbol{u}} - A^{-1}\mathbf{u}_N),$$

with relaxation parameters $\omega_i \in \mathbb{R}$. Optimization of these parameters with K41-theory can be found in Layton & Stanculescu (2007). The accelerated operators turn out to be self-adjoint and, if the relaxation parameters ω_i are positive, also positive definite.

Yosida. Another deconvolution operator, which is very common in the theory of semigroups or in the calculus of variations is the regularization coming from Yosida (1995), defined, for $\mu > 0$ by

$$\mathbf{u}_\mu := \frac{\mathrm{I} - (\mathrm{I} + \mu A)^{-1}}{\mu}\,\overline{\boldsymbol{u}}, \qquad \mu > 0.$$

To compare with the van Cittert operator we write the explicit expression for the symbol of the Yosida approximation in Fourier variables

$$\widehat{\mathrm{DY}}_\mu(\mathbf{k}) := (1 + \alpha^2 k^2)\frac{1}{\mu + \frac{1}{1+\alpha^2 k^2}}.$$

Tikhonov and Tikhonov–Lavrentiev. The classical Tikhonov method, see Tikhonov & Arsenin (1977), is based on the solution of a least squares method, with a regularization parameter $\mu > 0$. The approximate solution of $G\mathbf{u} = \overline{\boldsymbol{u}}$ is given by $\mathbf{u}_\mu$, which solves

$$\mathbf{u}_\mu := \operatorname*{argmin}_{\mu} \left[\|G\mathbf{u} - \overline{\boldsymbol{u}}\|^2 + \mu\|\mathbf{u}\|^2\right],$$

where we denote by $\|\,.\,\|$ the L^2-norm.

In case of a symmetric and positive-definite operator one can employ the Lavrentiev adaption and the Tikhonov–Lavrentiev regularization is given by the solution of the following minimization problem

$$\mathbf{u}_\mu := \operatorname*{argmin}_{\mu} \left[\frac{1}{2}(G\mathbf{u} - \overline{\boldsymbol{u}}, \mathbf{u}) + \frac{\mu}{2}\|\mathbf{u}\|^2\right];$$

by differentiation it follows that

$$\mathbf{u}_\mu = (\mu I + A^{-1})^{-1}\,\overline{\boldsymbol{u}}, \qquad 0 < \mu < 1.$$

For small wave numbers (large scales) this operator is not a good approximation of the operator A (and it is close to G^{-1} only for very small values of μ). By specifying the filter as the Helmholtz one, one obtains in Fourier variables

$$\widehat{\mathrm{DTL}}_\mu(\mathbf{k}) := (1 + \alpha^2 \mathrm{k}^2)\frac{1}{\mu + \frac{1}{1+\alpha^2 \mathrm{k}^2}},$$

i.e. exactly the same expression as the Yosida approximation.

Modified Tikhonov method. This method was introduced in Stanculescu & Manica (2010) and is designed for symmetric positive-definite operators. Given $\overline{\boldsymbol{u}}$ the approximate deconvolution solution $\mathbf{u}_\mu$ is defined by

$$\mathbf{u}_\mu := \big(\mu I + (1-\mu)A^{-1}\big)^{-1}\overline{\boldsymbol{u}}, \qquad 0 < \mu < 1.$$

We have the following expression for the operator in Fourier variables

$$\widehat{\mathrm{DMT}}_\mu(\mathbf{k}) := (1+\alpha^2 \mathrm{k}^2)\frac{1}{1-\mu+\mu(1+\alpha^2\mathrm{k}^2)}.$$

To better compare the deconvolution operators we set the parameter $\mu := (N+1)^{-1}$ and we have the expressions given in Table 1.1.

Deconvolution operator	Symbol in Fourier variables
$A = G^{-1}$	$(1+\alpha^2k^2)$
van Cittert	$(1+\alpha^2k^2)\left[1-\left(\frac{\alpha^2k^2}{(1+\alpha^2k^2)}\right)^{N+1}\right]$
Tikhonov–Lavrentiev & Yosida	$(1+\alpha^2k^2)\frac{N+1}{N+1+(1+\alpha^2k^2)}$
Modified Tikhonov	$(1+\alpha^2k^2)\frac{N+1}{N+1+\alpha^2k^2}$

Table 1.1 *Comparison of deconvolution operators for $\mu := (N+1)^{-1}$.*

Moreover, in all cases we have the following asymptotic expression.

Lemma 1.2.2 *For $\mu = (N+1)^{-1}$, with $N \in \mathbb{N}$, each of the four deconvolution operators (denoted generically by D_N) maps $\mathbf{H}^s$ into $\mathbf{H}^s$, is self-adjoint, commutes with differentiation, and*

$$\begin{aligned}
&\frac{N+1}{N+2} \le \widehat{D}_N(\mathbf{k}) \le N+1 && \forall\, \mathbf{k} \in \mathcal{T},\ \alpha > 0,\\
&\lim_{k\to+\infty} \widehat{D}_N(\mathbf{k}) = N+1 && \textit{for fixed } \alpha > 0,\\
&\widehat{D}_N(\mathbf{k}) \le (1+\alpha^2k^2) && \forall\, \mathbf{k} \in \mathcal{T},\ \alpha > 0.
\end{aligned}$$

In the cases of the van Cittert and of the modified Tikhonov schemes we also have the estimate $1 \le \widehat{D}_N(\mathbf{k}) \le N+1$. By direct inspection the van Cittert one is closer to the operator without deconvolution. We also observe that, beside the four operators we presented, other deconvolution operators have been recently introduced and analysed, for

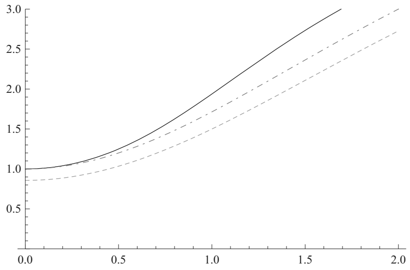

Figure 1.1 For $N = 5$, asymptotics near the origin. Solid for van Cittert, dashed for Tikhonov–Lavrentiev, and dash-dotted for modified Tikhonov.

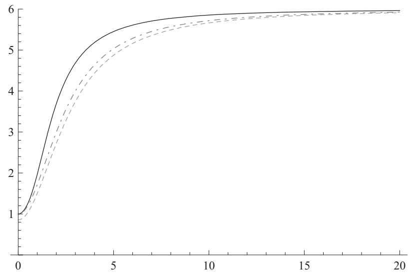

Figure 1.2 For $N = 5$, asymptotics for large wave numbers. Solid for van Cittert, dashed for Tikhonov–Lavrentiev, and dash-dotted for modified Tikhonov.

example, see Lewandowski (2009) for applications to some LES problems. In particular, the *continuous* deconvolution operator introduced in Bennis, Lewandowski, & Titi (2009) is defined by observing an analogy between the van Cittert algorithm and a finite difference equation, and by replacing discrete quantities with continuous ones.

1.3 High accuracy deconvolution alpha-models

In this section we introduce some LES models which are obtained from (1.2), (1.3), and (1.4) when introducing a deconvolution operator. Here D_N can be any of the deconvolution operators introduced in the previous section. Generally the theory is specialized for the van Cittert one but, being based on asymptotic properties of the operator, it can be adapted