

THE INTERIOR ERROR OF VAN CITTERT DECONVOLUTION OF DIFFERENTIAL FILTERS IS OPTIMAL

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Abstract. We reconsider the error in van Cittert deconvolution. We show that without any extra boundary conditions on higher derivatives of u , away from the boundary the error in van Cittert deconvolution of differential filters attains the high order of accuracy seen in the periodic problem. This error result is important for differential filters and approximate deconvolution models of turbulence.

This is an expanded version, containing more detail, background and supplementary material, of a report with the same title.

Key words. van Cittert deconvolution, singular perturbation, differential filters

1. Introduction. We consider the error in van Cittert deconvolution. We show that without any extra boundary conditions on higher derivatives of u , away from the boundary the error in van Cittert deconvolution attains the high order of accuracy seen in the periodic problem. The filtering problem is: given a function $u(x)$ defined on a domain Ω , compute an approximation $\bar{u}(x)$ to $u(x)$ which faithfully represents the behavior of u on scales above some, user selected, filter length (here denoted ε), and which truncates scales smaller than $O(\varepsilon)$. The deconvolution or de-filtering problem is: given \bar{u} find an accurate reconstruction of u . When the filter is smoothing $G : L^2(\Omega) \rightarrow L^2(\Omega)$ by $u \rightarrow \bar{u}$, G is compact and the deconvolution problem is ill-posed. One early method of deconvolution is the 1934 van Cittert [vC31] algorithm:

ALGORITHM 1.1 (van Cittert approximate deconvolution). *Set $u_0 = \bar{u}$. Fix N (moderate). For $n = 1, 2, \dots, N - 1$, perform*

$$u_{n+1} = u_n + \{\bar{u} - Gu_n\}$$

Define $D_N \bar{u} := u_N$.

REMARK 1.2. *The N^{th} van Cittert approximate deconvolution operator D_N is defined by N steps of Picard/ first order Richardson iteration for solving the operator equation $Gu = \bar{u}$ involving a possibly non-invertible operator G , [BB98]:*

given \bar{u} solve $Gu = \bar{u}$ for u .

by N steps of: $u_0 = \bar{u}$ and $u_{\text{new}} = u_{\text{old}} + \{\bar{u} - Gu_{\text{old}}\}$

Since the deconvolution problem is ill-posed, convergence as $N \rightarrow \infty$ cannot be expected. The relevant question is convergence for fixed N as $\varepsilon \rightarrow 0$.

The N^{th} van Cittert deconvolution operator D_N is given explicitly by

$$D_N \phi := \sum_{n=0}^N (I - G)^n \phi. \tag{1.1}$$

The van Cittert approximate deconvolution operator corresponding to $N = 0, 1, 2$ and their formal orders of accuracy with the differential filter (1.1) below are:

$$D_0 \bar{u} = \bar{u} = u + O(\varepsilon^2),$$

$$D_1 \bar{u} = 2\bar{u} - \bar{\bar{u}} = u + O(\varepsilon^4),$$

$$D_2 \bar{u} = 3\bar{u} - 3\bar{\bar{u}} + \bar{\bar{\bar{u}}} = u + O(\varepsilon^6).$$

Van Cittert deconvolution thus requires only a few steps of repeated filtering. It is thus both computationally cheap and easy to program, contributing to its popularity in various applications, such as turbulence modeling, e.g., [LR12]. For convolution filters and under periodic boundary conditions, the error in van Cittert can be analyzed precisely by Fourier methods, e.g., [BIL06], [D04], [DE06]. In other cases there are significant gaps between the improved accuracy seen in computational practice and the pessimistic estimates of its global error obtained in analysis.

The goal of this report is to close this gap somewhat. We give error estimates for the van Cittert deconvolution under nonperiodic boundary conditions and preserving the boundary conditions. To develop these local and global estimates we must focus on a specific problem. To begin, we take the filter to be a differential filter (Germano [Ger86]) specifically the extension of the Pao filter, e.g., [Po00], to a bounded domain. Let Ω be a bounded, regular, planar domain with smooth boundary and $0 < \varepsilon \leq 1$ a small parameter. Given $u \in H_0^1(\Omega)$, define $Gu = \bar{u}$ as the unique solution of the elliptic-elliptic singular perturbation problem

$$-\varepsilon^2 \Delta \bar{u} + \bar{u} = u, \text{ in } \Omega, \text{ and } \bar{u} = 0, \text{ on } \partial\Omega. \quad (1.2)$$

Classical theory, [L73], concludes that

$$\bar{u} \rightarrow u \text{ in } L^2(\Omega) \text{ as } \varepsilon \rightarrow 0.$$

This can be extended to $\bar{u} \rightarrow u$ in $H_0^1(\Omega)$ as $\varepsilon \rightarrow 0$, [L07]. Further, the shift theorem implies that $\bar{u} \in H_0^1(\Omega) \cap H^3(\Omega)$. Since traces of $\Delta \bar{u}$ are thus well defined, $-\varepsilon^2 \Delta \bar{u} + \bar{u} = u$ implies

$$\bar{u} = 0 \text{ and } \Delta \bar{u} = 0 \text{ on } \partial\Omega.$$

As an example of the difficulties connected with the global error, consider the case $N = 0$ (no deconvolution) and $N = 1$. The regularity theory (sharp in 1d examples [L07]) predicts no improvement in the rate of convergence in L^2 , whose norm is denoted $\|\cdot\|$. We prove the following herein which predicts improvement from higher order deconvolution in negative Sobolev norms and away from the boundary.

THEOREM 1.3 (Global and Local Deconvolution Errors). *Suppose $N > 0$ is fixed and for k large enough that $u \in H^k(\Omega) \cap H_0^1(\Omega)$. Then*

$$\|u - D_0 \bar{u}\| = \|u - \bar{u}\| \leq C\varepsilon^2 \|u\|_{H^2(\Omega)}$$

If $N = 1$ we have in L^2 and H^{-2}

$$\|u - D_1 \bar{u}\| \leq C\varepsilon^2 \|u\|_{H^2(\Omega)} \quad \text{and} \quad \|u - D_1 \bar{u}\|_{H^{-2}(\Omega)} \leq C\varepsilon^4 \|u\|_{H^2(\Omega)}$$

If $N = 1$ and additionally $\Delta u \in H_0^1(\Omega)$

$$\|u - D_1 \bar{u}\| \leq C\varepsilon^4 \|u\|_{H^2(\Omega)}$$

If $\Delta u \neq 0$ on $\partial\Omega$ we have

$$\begin{aligned} \|u - D_N \bar{u}\| &\leq C\varepsilon^2 \|u\|_{H^2(\Omega)} \\ \|u - D_N \bar{u}\|_{H^{-2N}(\Omega)} &\leq C\varepsilon^{2N+2} \|u\|_{H^2(\Omega)}. \end{aligned}$$

Let $s \geq 0$. Suppose $u \in H^{2N+2}(\Omega) \cap H_0^1(\Omega)$. Let

$$\Omega_{N+1} \subset \Omega_N \subset \cdots \subset \Omega_1 \subset \Omega_0 \subset \Omega_{-1} \equiv \Omega$$

be subdomains with smooth boundaries and for $j = N + 1, \dots, 0$ with

$$\Omega_j \text{ has distance } C_j \varepsilon \ln(1/\varepsilon) \text{ from } \partial\Omega_{j-1},$$

where $C_j = C(s, N, \Omega_j, \Omega_{j-1})$. Then there is a $C = C(N, C_j)$ such that

$$\|u - D_N \bar{u}\|_{L^2(\Omega_{N+1})} \leq C \varepsilon^{2N+2} [\|u\|_{H^{2N+2}(\Omega_0)} + \varepsilon^s \|u\|]$$

1.1. The case of local averaging filters. If the filter is a local averaging filter then interior estimates of the above type hold automatically because the calculation of $\bar{\phi}$ on Ω_j only accesses the values of ϕ on Ω_{j-1} . Local averaging filter are vevry important in finite difference methods. Three examples follow.

Top hat filter. The top hat filter is the un-weighted average defined over a neighborhood of a given point:

$$B_\delta(x) := \{y : |x - y| < \varepsilon\},$$

$$\bar{u}(x) := \frac{1}{\text{vol}(B_\varepsilon(x))} \int_{B_\varepsilon(x)} u(y) dy.$$

Thus in 3d this means

$$\bar{u}(x) := \frac{1}{\frac{4}{3}\pi\varepsilon^3} \int_{|x-y|<\varepsilon} u(y) dy.$$

This can be written as a convolution by choosing $g_\delta(x) := \varepsilon^{-3}g(x/\varepsilon)$ where

$$g(x) = 1, \text{ if } |x| < \frac{3}{4\pi},$$

$$g(x) = 0, \text{ if } |x| \geq \frac{3}{4\pi}.$$

Discrete filters. In finite difference approximations, ultimately one must filter discrete velocities defined on a finite difference mesh. On a uniform mesh in 2d with averaging radius equal to the given meshwidth, $\varepsilon = \Delta x$, using the standard finite difference compass notation the analog of the top hat filter is

$$\bar{u}(P) := \frac{u(N) + u(S) + u(E) + u(W) + u(P)}{5}$$

Weighted Compact Discrete Filter, [SAK01a]. There has developed a considerable experience with weighted discrete filters inspired by the needs of difference methods. On structured meshes, filters can be derived in 1d and extended by taking tensor products of 1d filters. Generally, the higher order the filter, the more points involved in the averaging operator and thus the greater the bandwidth on the linear system that must be solved. Compact filters are a clever idea of Stolz, Adams and Kleiser [SAK01a]; they attain higher order but only require tridiagonal solves (on structured meshes). The following 1d weighted discrete filter from [SAK01a] has second order accuracy and has proven its value in large eddy simulation. Given values

u_i of the variable u at equi-spaced mesh points x_i , a weighting parameter α is chosen in the range $-1/2 \leq \alpha \leq +1/2$. Then, filtered values are calculated by solving the tridiagonal system

$$\alpha \bar{u}_{i-1} + \bar{u}_i + \alpha \bar{u}_{i+1} = \left(\frac{1}{2} + \alpha\right) \left(u_i + \frac{u_{i-1} + u_{i+1}}{2}\right).$$

The fact that the inverse of a tridiagonal matrix is a full matrix means that local error estimates for van Cittert deconvolution do not follow automatically for weighted compact filters. This extension is an open problem.

2. Proof of the deconvolution error estimate. Since van Cittert deconvolution is mathematically equivalent to a truncation of a geometric (operator) series, it is quite easy to calculate the deconvolution error for specific choices of filter for smooth functions. The error in van Cittert deconvolution is thus calculated, [BIL06], [D04], [DE06], to be

$$\begin{aligned} u - D_N \bar{u} &= (I - G)^{N+1} u = (-1)^{N+1} \varepsilon^{2N+2} \Delta^{N+1} G^{N+1} u \\ &= O(\varepsilon^{2N+2}) \text{ for } C_{\text{periodic}}^\infty \text{ functions } u. \end{aligned} \quad (2.1)$$

Thus, accuracy of van Cittert in any norm $||| \cdot |||$ depends on whether, and for what values on N ,

$$||| \Delta^{N+1} G^{N+1}(u) ||| \leq C(u) < \infty \text{ uniformly in } \varepsilon.$$

The proof is based on the error representation (2.1) and two regularity results for the elliptic-elliptic singular perturbation problem. The global regularity result was proven in [L07], see also [LR12]. The local, interior regularity result is a special case of Theorem 2.3, page 26 of Navert [N82] (setting the convecting velocity to zero), see also [SW83]. We shall first recall these two results, give a preliminary lemma and then give the proof (which is short with this preparation). $H^k(\Omega)$ denotes the Sobolev space of all functions with derivatives of order $\leq k$ in $L^2(\Omega)$. The $L^2(\Omega)$ norm is $\|\cdot\|$ and $H_0^1(\Omega) := \{v \in H^1 : v = 0 \text{ on } \partial\Omega\}$. For (1.1) we assume (in particular implying $u = 0$ on $\partial\Omega$)

$$u \in H^k(\Omega) \cap H_0^1(\Omega). \quad (2.2)$$

This condition precludes simple boundary layers in \bar{u} but does not imply higher derivatives of \bar{u} are free of layers. From (1.1) it also implies that $\Delta \bar{u} = 0$ on $\partial\Omega$.

THEOREM 2.1 (Theorem 1.1 in [L07]). *Suppose $u \in H^2(\Omega) \cap H_0^1(\Omega)$. Then there is a constant $C > 0$ independent of ε such that*

$$\|\bar{u}\|_{H^l(\Omega)} \leq C \|u\|_{H^l(\Omega)}, \text{ for } l = 0, 1, 2. \quad (2.3)$$

If $u \in H^4(\Omega) \cap H_0^1(\Omega)$, $\Delta u \in H_0^1(\Omega)$. Then

$$\|\bar{u}\|_{H^l(\Omega)} \leq C \|u\|_{H^l(\Omega)}, \text{ for } l = 0, 1, 2, 3, 4. \quad (2.4)$$

In general, suppose $u \in H^{2k}(\Omega) \cap H_0^1(\Omega)$, $\Delta^j u \in H_0^1(\Omega)$, $j = 1, \dots, k-1$. Then for $l = 1, \dots, 2k$

$$\|\bar{u}\|_{H^l(\Omega)} \leq C \|u\|_{H^l(\Omega)}. \quad (2.5)$$

Examples in [L07] show that the estimate $\|\bar{u}\|_l \leq C\|u\|_l$, being limited to $l = 0, 1, 2$ is sharp unless higher derivatives of u are zero on $\partial\Omega$.

THEOREM 2.2 (Special case of Navert [N82], Theorem 2.3). *For $u \in H^k(\Omega) \cap H_0^1(\Omega)$ consider*

$$-\varepsilon^2 \Delta \bar{u} + \bar{u} = u, \text{ in } \Omega, \text{ and } \bar{u} = 0, \text{ on } \partial\Omega. \quad (2.6)$$

Let $m \geq 0, s \geq 0$. Let $\Omega' \subset \Omega'' \subset \Omega$ be subdomains with smooth boundaries with

- Ω' has distance $C_1 \varepsilon \ln(1/\varepsilon)$ from $\partial\Omega''$,
- Ω'' has distance $C_2 \varepsilon \ln(1/\varepsilon)$ from $\partial\Omega$.

where $C_i = C_i(s, m, \Omega', \Omega'')$. Then the solution to (1.1) satisfies

$$\|\bar{u}\|_{H^m(\Omega')} \leq C (\|u\|_{H^m(\Omega'')} + \varepsilon^s \|u\|)$$

First we calculate the global regularity of repeated filtering.

PROPOSITION 2.3. *Let $u \in H^k(\Omega) \cap H_0^1(\Omega)$. We have for $J \geq 1$*

$$\|G^J u\|_{H^k(\Omega)} \leq C \|G^{J-1} u\|_{H^k(\Omega)}, k = 0, 1, \dots, 2J.$$

Proof. For $n = 1$ Theorem 1.1 implies

$$\|\bar{u}\|_{H^k(\Omega)} \leq C \|u\|_{H^k(\Omega)}, \text{ for } k = 0, 1, 2 \text{ and } \Delta \bar{u} = 0 \text{ on } \partial\Omega.$$

Since $\Delta \bar{u} = 0$ on $\partial\Omega$, we repeat. Indeed, $G^2 u = G\bar{u} = \bar{\bar{u}}$ so that

$$\begin{aligned} \|\bar{\bar{u}}\|_{H^k(\Omega)} &\leq C \|\bar{u}\|_{H^k(\Omega)}, \text{ for } k = 0, 1, 2, 3, 4 \text{ and that} \\ \Delta \bar{\bar{u}} &= \Delta \bar{u} = 0 \text{ on } \partial\Omega. \end{aligned}$$

Taking the Laplacian of the equation for $\bar{\bar{u}}$ gives

$$-\delta^2 \Delta^2 \bar{\bar{u}} + \Delta \bar{\bar{u}} = \Delta \bar{u}, \text{ in } \Omega. \quad (2.7)$$

Now, let $x \rightarrow \partial\Omega$ and use $\Delta \bar{\bar{u}} = \Delta \bar{u} = 0$ on $\partial\Omega$. This implies

$$\Delta^2 \bar{\bar{u}} = \Delta \bar{\bar{u}} = \bar{\bar{u}} = 0 \text{ on } \partial\Omega$$

so that for $\bar{\bar{\bar{u}}}$.

$$\|\bar{\bar{\bar{u}}}\|_{H^k(\Omega)} \leq C \|\bar{\bar{u}}\|_{H^k(\Omega)}, \text{ for } k = 0, 1, 2, 3, 4, 5, 6.$$

The proof continues by induction. \square

We can now prove the deconvolution error estimate in Theorem 1.1.

Proof. [Proof of Theorem 1.1] We consider $\Delta^{N+1} G^{N+1}(u)$ and use Theorem 1.1 in [L07] repeatedly. For $N = 0$ this is $\|\Delta(-\varepsilon^2 \Delta + 1)^{-1} u\|$:

$$\|u - D_0 \bar{u}\| = \|u - \bar{u}\| = \varepsilon^2 \|\Delta(-\varepsilon^2 \Delta + 1)^{-1} u\|.$$

The first estimate follows since:

$$\|\Delta(-\varepsilon^2 \Delta + 1)^{-1} u\| = \|\Delta \bar{u}\| \leq C \|\bar{u}\|_2 \leq C \|u\|_2$$

For $N = 1$ and under $\Delta u \in H_0^1(\Omega)$ we have similarly that $\|\bar{u}\|_4 \leq C\|u\|_4$. Thus

$$\|u - D_1 \bar{u}\| = \varepsilon^4 \|\Delta^2 \bar{u}\| \leq C\varepsilon^4 \|\bar{u}\|_4 \leq C\varepsilon^4 \|u\|_4.$$

For the H^{-2} estimate we use that $\Delta^2 \bar{u} = \Delta(\overline{\Delta u})$. Step by step, using $\Delta \bar{u} = 0$ on $\partial\Omega$ we find $\|\Delta^2 \bar{u}\|_{-2} \leq C\|\overline{\Delta u}\| \leq C\|\Delta u\| \leq C\|u\|_2$, completing the proof. The case of $N > 1$ follows the same way.

For the interior estimates we use Theorem 2.2 as follows.

$$\begin{aligned} \|u - D_N \bar{u}\|_{L^2(\Omega_{N+1})} &= \varepsilon^{2N+2} \|(\Delta^{N+1} G^{N+1})u\|_{L^2(\Omega_{N+1})} \leq \\ &\leq C\varepsilon^{2N+2} \|G^{N+1}u\|_{H^{2N+2}(\Omega_{N+1})}. \end{aligned}$$

Note that $\|\bar{\phi}\| \leq \|\phi\|$ so that $\|G^j u\| \leq \|u\|$ for all j . Now $G^{N+1}u = \bar{\phi}$, $\phi = G^N u$. Thus, for any $s > 0$

$$\begin{aligned} \|G^{N+1}u\|_{H^{2N+2}(\Omega_{N+1})} &\leq C (\|G^N u\|_{H^{2N+2}(\Omega_N)} + \varepsilon^s \|G^N u\|) \\ &\leq C (\|G^N u\|_{H^{2N+2}(\Omega_N)} + \varepsilon^s \|u\|). \end{aligned}$$

We repeat this argument. Indeed, $G^N u = \bar{\phi}$, $\phi = G^{N-1}u$. Thus, for any $s > 0$

$$\|G^N u\|_{H^{2N+2}(\Omega_N)} \leq C (\|G^{N-1}u\|_{H^{2N+2}(\Omega_{N-1})} + \varepsilon^s \|u\|).$$

At the last step we have, for any $s > 0$

$$\|G^1 u\|_{H^{2N+2}(\Omega_1)} \leq C (\|u\|_{H^{2N+2}(\Omega_0)} + \varepsilon^s \|u\|).$$

Thus (recalling that N is fixed and C can depend on N) we have

$$\|u - D_N \bar{u}\|_{L^2(\Omega_{N+1})} \leq C\varepsilon^{2N+2} [\|u\|_{H^{2N+2}(\Omega_0)} + \varepsilon^s \|u\|]$$

□

3. Conclusions. The filtering or convolution operator $G : u \rightarrow \bar{u}$ is a bounded map: $L^2(\Omega) \rightarrow L^2(\Omega)$. If (as for differential filters) it is smoothing, its inverse cannot be bounded due to small divisor problems. Indeed, it is known quite generally that inversion is not well posed.

THEOREM 3.1. *Let H be a Hilbert space and $G : H \rightarrow H$ a compact map. Then, if H is infinite dimensional*

$$\text{Range}(G) \neq H.$$

In other words, G is not invertible as a bounded linear operator.

Thus stable exact deconvolution is not possible and approximate deconvolution must be used instead. An approximate deconvolution operator D_N is an approximate inverse $\bar{u} \rightarrow D_N(\bar{u}) \approx u$ which

- is a bounded operator on $L^2(\Omega)$,
- approximates u in some useful (typically asymptotic) sense, and
- satisfies other conditions necessary for the application at hand.

The error in *van Cittert approximate deconvolution* in the non periodic case is of high accuracy, away from boundaries, like that of the periodic case. It is an interesting analytic open question to establish if a similar result holds for the Stokes differential filter. It is also an interesting algorithmic open question to alter the van Cittert procedure near boundaries to obtain a high order accurate reconstruction of the unknown function up to the boundary.

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3.1. More References to work on approximate deconvolution models in CFD.

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