

Analytic continuation of Dirichlet-Neumann operators

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Summary. The analytic dependence of Dirichlet-Neumann operators (DNO) with respect to variations of their domain of definition has been successfully used to devise diverse computational strategies for their estimation. These strategies have historically proven very competitive when dealing with small deviations from exactly solvable geometries, as in this case the perturbation series of the DNO can be easily and recursively evaluated. In this paper we introduce a scheme for the enhancement of the domain of applicability of these approaches that is based on techniques of analytic continuation. We show that, in fact, DNO depend analytically on variations of *arbitrary* smooth domains. In particular, this implies that they generally remain analytic beyond the disk of convergence of their power series representations about a canonical separable geometry. And this, in turn, guarantees that alternative summation mechanisms, such as Padé approximation, can be effectively used to numerically access this extended domain of analyticity. Our method of proof is motivated by our recent development of *stable* recursions for the coefficients of the perturbation series. Here, we again utilize this recursion as we compare and contrast the performance of our new algorithms with that of previously advanced perturbative methods. The numerical results clearly demonstrate the beneficial effect of incorporating analytic continuation procedures into boundary perturbation methods. Moreover, the results also establish the superior accuracy and applicability of our new approach which, as we show, allows for precise calculations corresponding to very large perturbations of a basic geometry.

1 Introduction

Many fundamental problems in mathematical physics are phrased in terms of partial differential equations posed on irregular or moving domains. While, in many cases, the equations governing quantities in the interior of the domain may be simple (linear, and even constant coefficient), the geometrical complexity of the boundary and/or nonlinearities in the boundary conditions generally render these problems analytically intractable. This is the case, for instance, for standard boundary value problems such as those arising in scattering models associated with irregular obstacles (see e.g. [3]), or for classical free boundary problems such as those modeling water waves, Hele-Shaw flows [15], precipitate growth, and solid-liquid phase transformations [12]. It is a general principle of the aforementioned problems that a simplification and reduction in dimension can be accomplished by considering the field quantities evaluated at the boundary and, if applicable, the shape of the boundary itself, as fundamental variables. From these boundary variables the field quantities can be recovered from suitable representation formulas. Generally, a complication in such a reduction is that normal derivatives of the fields at the boundary of their domain of definition may be required (to enforce continuity of electromagnetic quantities, or kinematic/dynamic compatibility, or conservation of energy, etc). Such requirements then demand that Dirichlet-Neumann operators (DNO), and their higher order analogues, enter into these surface formulations to relate boundary values (“Dirichlet data”) to normal derivatives (“Neumann data”).

From a computational perspective, the above reduction procedure makes the accurate and stable estimation of DNO essential. Among the myriad of methods that can be devised for the numerical approximation of DNO, boundary perturbation methods present an appealing alternative within their regime of relevance. These methods are based on the observation that for certain (“separable”) simple geometries, DNO can be explicitly constructed. Thus, a perturbation series in powers of a parameter measuring deviation from such a geometry can be effectively obtained through the recursive solution of a sequence of relatively simple problems. A particularly attractive feature of these methods is that, in contrast with alternative approaches (e.g. finite elements or surface potentials), their implementation and performance do not depend strongly on the spatial dimension. In fact, it has been shown that perturbation methods can lead very efficiently to highly accurate results for small to moderate perturbations of two- and three-dimensional separable geometries, see e.g. [10, 16, 17, 20, 21, 9, 14, 19, 18, 27]. For large deformations, on the other hand, these implementations are limited by the radius of convergence of the perturbation series. In this paper we address this very issue, as we introduce a scheme for the enhancement of the domain of applicability of boundary perturbation approaches that is based on techniques

of analytic continuation. We show that, in fact, DNO depend analytically on variations of *arbitrary* smooth domains (see Sect. 3). In particular, this implies that they generally remain analytic beyond the disk of convergence of their power series representations about a canonical geometry. And this, in turn, guarantees that alternative mechanisms for summation of Taylor series, such as Padé approximation, can be effectively used to numerically access this extended domain of analyticity (corresponding to large deformations; see Sect. 5). As we demonstrate, the incorporation of these analytic continuation techniques substantially improves the overall performance of algorithms based on boundary variations.

The extended analyticity theorems for DNO that we present in Sect. 3 and 4 are in the spirit of the results in [3] where similar properties were shown to hold for solutions to (exterior) scattering problems. In [3] these properties were established through a careful inversion in a space of holomorphic functions of an appropriate integral equation formulation. Our method of proof is quite different and, in fact, more direct and generally applicable, as it is based on the inductive estimation of suitable recurrences for the Taylor coefficients of the field quantities. In particular, and as we show in Sect. 4, a simple extension of our arguments delivers an alternative proof of the exact analogue of the results in [3], namely that of *joint* analyticity of the fields in spatial variables and variation parameter.

As we said, the recurring nature of the formulas for the coefficients in a representation of the DNO in powers of a boundary roughness parameter constitutes a main ingredient in perturbative approaches. And, in fact, several implementations of these recursions have been proposed. In the context of simulations of gravity water waves, for instance, the early work of Dommermuth and Yue [10] advocated the expansion of the field (i.e. the velocity potential) in powers of the water's surface elevation and the subsequent evaluation of its normal derivative (normal velocity). In contrast, and still within the context of water waves, Craig and Sulem [9] later on devised a recursion that applies to the DNO itself and thus directly produces the normal velocity at the surface from the values of the potential there (see also [26, 23, 22, 7]). Their scheme, in fact, closely resembles that introduced earlier by Milder [16, 17] (see also [20, 21, 14, 19, 18, 27]) in his studies of electromagnetic ocean scattering. Interestingly, we have recently shown [24] that none of these procedures produces recursions that are suitable for an inductive estimation that would lead to a proof of analyticity of DNO. Indeed, we have demonstrated that both the "field expansion" (FE) approach of [10] and the "operator expansion" (OE) method of [9, 16, 17] result in recursions that contain cancellations and, thus, lead to rather unstable numerics (see Sect. 2). From a theoretical standpoint, these cancellations conspire against a straightforward estimation of the terms in the series. In [24] we resolved this

problem by introducing yet another set of recursive formulas for the Taylor series of the DNO, leading to what we termed the method of “transformed field expansions” (TFE). These formulas, which are obtained after a change of variables is effected that transforms the perturbed domain onto the unperturbed geometry, can be shown to be free of cancellations and were used in [24] to establish the analyticity of DNO for small boundary perturbations. Here, we again utilize this idea to establish the analytic continuation results mentioned above.

The paper is organized as follows: first, and for the sake of completeness, we review, in Sect. 2, the basic concepts relating to perturbation methods as applied to the approximation of DNO. We further introduce the FE and OE implementations and we demonstrate their rather unstable behavior, due to the presence of strong cancellations in the associated recursions. In Sect. 3 we introduce our new recurrence based on collapsing the perturbed domains onto the unperturbed geometry. We show that, in contrast with those arising in the OE and FE schemes, these formulas can in fact be used to establish the analyticity of DNO for perturbations of an arbitrary (smooth) domain. A similar, though slightly more subtle, argument is presented in Sect. 4 that shows that, for analytic perturbations, the field is in fact *jointly* analytic in spatial variables and perturbation parameter. Finally, in Sect. 5, we present a variety of numerical results that demonstrate the beneficial effect of incorporating analytic continuation mechanisms into perturbative approaches as we compare the OE and FE schemes with our new TFE method. These results also establish the superior accuracy and applicability of TFE which, as we show, allows for precise calculations corresponding to very large perturbations of a basic geometry.

2 Perturbative methods for evaluation of DNO

In this section we review the fundamental ideas underlying the perturbative expansion of DNO as we introduce the recursive formulas that constitute the basis of the various implementations of these approximation schemes. Clearly, the details of these recurrences will depend upon the physical model under consideration, its natural characteristics, and geometrical features. For the sake of definiteness, and for ease of comparison with prior work, here we shall consider a model that arises in the study of water waves [10,9] and which leads to the DNO associated with a (periodic) rectangular geometry. As will be evident, our results apply more generally to perturbations of any exactly solvable geometry. More precisely, we shall consider

$$(1) \quad S_\sigma = \{(x, y) \in \mathbf{R}^{d-1} \times \mathbf{R} \mid -1 < y < \sigma(x)\}$$

and the unique solution, v , of the problem

$$\begin{aligned}
 (2a) \quad & \Delta v = 0 && \text{in } S_\sigma \\
 (2b) \quad & v(x, \sigma(x)) = \xi(x) \\
 (2c) \quad & \partial_y v(x, -1) = 0 \\
 (2d) \quad & v(x + \gamma, y) = v(x, y) && \text{for all } \gamma \in \Gamma
 \end{aligned}$$

where $\Gamma \subset \mathbf{R}^{d-1}$ is a lattice of periodicity. Then the Dirichlet-Neumann operator, $G(\sigma)$, is defined as

$$(3) \quad G(\sigma) \xi = \nabla v|_{y=\sigma} \cdot (-\nabla_x \sigma, 1)^T.$$

We remark that the above definition could be based upon a domain of any depth h (i.e. $-h < y < \sigma(x)$) or even of infinite depth ($-\infty < y < \sigma(x)$) by suitably adjusting (2c), e.g. for infinite depth by enforcing

$$(4) \quad \partial_y v(x, y) \rightarrow 0 \quad \text{as } y \rightarrow -\infty.$$

The accurate numerical evaluation of DNO is evidently a nontrivial matter as it entails, directly or indirectly, the approximation of singular integrals (see e.g. [8]). There is, however, one exception: for a separable geometry, the operator can be explicitly found. In our case, such a geometry is provided by a “flat ocean”, corresponding to $\sigma = 0$. Indeed, in this case, we have

$$(5) \quad G(0) \xi = |D| \tanh(|D|) \xi(x) = \sum_{k \in \Gamma'} |k| \tanh(|k|) \hat{\xi}(k)$$

for a domain of unit depth (c.f. (1)), or

$$(6) \quad G(0) \xi = |D| \xi(x) = \sum_{k \in \Gamma'} |k| \hat{\xi}(k)$$

for a domain of infinite depth, where $D = -i\nabla_x$ and Γ' is the conjugate lattice to Γ (i.e. wavenumbers). In view of this, a perturbative approach suggests itself whereby a general surface is viewed as a deviation from a plane. More precisely, a family of surfaces $\sigma = \varepsilon f$, $|\varepsilon| \leq \bar{\varepsilon}$, gives rise to DNO, $G(\varepsilon f)$, and a perturbation series

$$(7) \quad G(\varepsilon f) \xi = \sum_{n=0}^{\infty} (G_n(f) \xi) \varepsilon^n$$

could be used for their approximation. The feasibility of such an approach obviously hinges on two main factors: 1) the convergence of the series (7), and 2) the development of an algorithm for the efficient evaluation of its coefficients.

The question of convergence of the series (7) has a long history and, for two-dimensional domains (i.e. $d = 2$), an affirmative answer can be derived from the work of Calderón [4] and Coifman and Meyer [5]. Indeed, it follows from these that for any Lipschitz profile f there exists a constant $B > 0$ such that

$$(8) \quad \|G_n(f) \xi\|_{L^2} \leq C \|\xi\|_{H^1} B^n$$

which implies that the series (7) converges in L^2 for sufficiently small values of ε . Extensions of these results to higher dimensions were recently established by Craig, Schanz, and Sulem [8] and Craig and Nicholls [6] (see also Nicholls and Reitich [24]).

As for the numerical evaluation of the Taylor coefficients $G_n(f)$ in (7), the perturbative nature of the series implies that, at least formally, they can be *recursively* obtained. In the next section we review two implementations of these recursions that have been previously proposed. As we explain in Sect. 2.2 these algorithms, though very efficient, are somewhat limited by their conditioning properties.

2.1 The field expansion and operator expansion methods

A natural approach to the perturbative approximation of DNO, which we shall refer to as the method of Field Expansions (FE), consists of simply expanding the *field* $v = v(x, y, \varepsilon)$ solving Eqn. (2) (or (2) with (2c) replaced by (4)), for $\sigma(x) = \varepsilon f(x)$, in the form

$$(9) \quad v(x, y, \varepsilon) = \sum_{n=0}^{\infty} v_n(x, y) \varepsilon^n$$

and, a posteriori, of computing the DNO based on this expansion via the formula

(10)

$$G_n(f) \xi = -\nabla_x f \cdot \sum_{l=0}^{n-1} \frac{f^l}{l!} \partial_y^l \nabla_x v_{n-1-l}(x, 0) + \sum_{l=0}^n \frac{f^l}{l!} \partial_y^{l+1} v_{n-l}(x, 0)$$

(see [10]). For instance, in the case of infinite depth (cf. (4)) it is easy to show that the functions $v_n(x, y)$ must satisfy

$$(11a) \quad \Delta v_n(x, y) = 0 \quad \text{in } S_0$$

$$(11b) \quad \partial_y v(x, y) \rightarrow 0 \quad \text{as } y \rightarrow -\infty$$

$$(11c) \quad v_n(x, 0) = H_n(x)$$

$$(11d) \quad v_n(x + \gamma, y) = v_n(x, y) \quad \text{for all } \gamma \in \Gamma$$

where

$$(12) \quad H_n(x) = - \sum_{l=0}^{n-1} \frac{f^{n-l}}{(n-l)!} \partial_y^{n-l} v_l(x, 0) + \delta_{n,0} \xi(x)$$

and $\delta_{j,k}$ is the Kronecker delta. A spectral representation of the solution of Eqns. (11a), (11b), (11d) is given by

$$(13) \quad v_n(x, y) = \sum_{k \in \Gamma'} d_{n,k} e^{ik \cdot x + |k|y}$$

where $d_{n,k}$ are Fourier coefficients. Eqn. (11c) then translates into the recursion

$$(14) \quad d_{n,k} = - \sum_{l=0}^{n-1} \sum_{q \in \Gamma'} C_{n-l, k-q} d_{l,q} |q|^{n-l} + \delta_{n,0} \hat{\xi}(k),$$

where the numbers $C_{l,k}$ are the Fourier coefficients of the function $f(x)^l/l!$, that is

$$(15) \quad \frac{f(x)^l}{l!} = \sum_{k \in \Gamma'} C_{l,k} e^{ik \cdot x}.$$

The formula (14) can be used to recursively evaluate the coefficients $d_{n,k}$ and these, in turn, allow for the calculation of the Fourier representation of $G_n(f)$ by means of equation (10).

An alternative and elegant scheme for the calculation of the operators $G_n(f)$ was proposed by Milder [16] in the context of ocean scattering and again by Craig and Sulem [9] in their study of gravity water waves. The method works directly with the DNO without reference to the bulk potential and has thus been termed the ‘‘Operator Expansion’’ (OE) method. To review this approach, let us assume again that the basic geometry is of infinite extent in y , in which case the unperturbed DNO is given by (6). Since the function

$$(16) \quad w_p(x, y) = e^{ip \cdot x + |p|y},$$

is a solution of (2a), (2d), (4) we have

$$(17) \quad G(\varepsilon f) \left[e^{ipx + |p|\varepsilon f} \right] = (\partial_y - \varepsilon \nabla_x f \cdot \nabla_x) (e^{ip \cdot x + |p|y}) \Big|_{y=\varepsilon f},$$

that is

$$(18) \quad G(\varepsilon f) \left[e^{ipx + |p|\varepsilon f} \right] = (|p| - \varepsilon \nabla_x f \cdot ip) e^{ip \cdot x + |p|\varepsilon f}.$$

Thus, expanding the equality (18) in the form of a series in ε and equating like powers we obtain the recursion

$$(19) \quad G_n(f)e^{ip \cdot x} = \frac{f^n}{n!} |p|^{n+1} e^{ip \cdot x} - (\nabla_x f) \frac{f^{n-1}}{(n-1)!} \cdot (ip) |p|^{n-1} e^{ip \cdot x} \\ - \sum_{l=0}^{n-1} G_l(f) \left[\frac{f^{n-l}}{(n-l)!} |p|^{n-l} e^{ip \cdot x} \right]$$

or, symbolically,

$$(20) \quad G_n(f) \xi(x) = D \frac{f^n}{n!} D |D|^{n-1} \xi(x) - \sum_{l=0}^{n-1} G_l(f) \left[\frac{f^{n-l}}{(n-l)!} |D|^{n-l} \xi(x) \right].$$

Finally, using the self-adjoint nature of $G_n(f)$ and $|D|$, we may rewrite (20) in the form

$$(21) \quad G_n(f) \xi(x) = |D|^{n-1} D \frac{f^n}{n!} D \xi(x) - \sum_{l=0}^{n-1} |D|^{n-l} \frac{f^{n-l}}{(n-l)!} G_l(f) \xi(x)$$

which gives a direct recurrence for the operators $G_n(f)$.

2.2 Cancellations and Ill-conditioning

It is important to note that the above derivations of (14) and (21) are formal in nature. Indeed, although the results in [4, 5, 8, 6, 24] do guarantee the convergence of the expansion (7), the validity of these recursions demands more careful consideration. In fact, at first glance the formulas would seem to require a high degree of regularity on the profile f , as is most evidently displayed in equation (21). On the other hand, the theoretical results on analyticity of DNO apply to general “rough” (Lipschitz or C^1) perturbations of a plane. As conjectured in [24] and demonstrated in [25], this apparent contradiction is at the heart of the unstable behavior of the OE and FE algorithms in high-order calculations. Indeed, as shown in [24, 25], substantial cancellations occur in (14) and (21) so that the overall sums in their respective right-hand-sides give rise to finite quantities in spite of possible singularities in the individual terms.

To motivate the need for a better conditioned approach let us consider here the case of *smooth* (one dimensional) perturbations of the plane $y = 0$ given by

$$f(x) = 2 \cos(x)$$

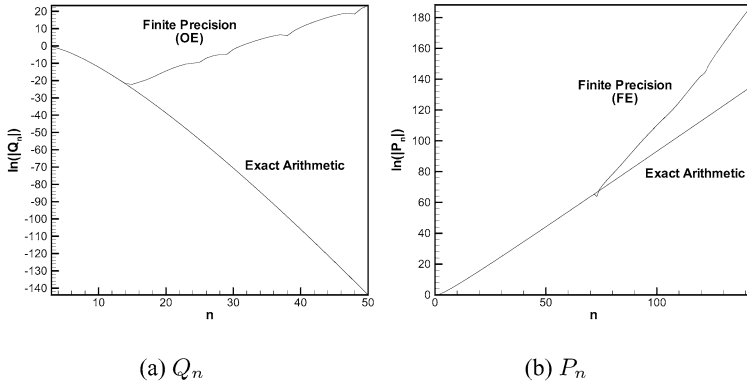


Fig. 1. Computation of Q_n and P_n in finite precision and exact arithmetic

with Dirichlet data

$$\xi(x) = 2 \cos(x).$$

In this case, calculations in *exact* (rational) arithmetic can be performed by resorting to a symbolic manipulator (Maple, in our case) with rather modest memory and time requirements. In this manner the precise values of the Fourier coefficients $d_{n,k}$ (cf. (14)) and those of $a_{n,k}$ corresponding to the (periodic) functions

$$G_n(f) \xi = \sum_{k \in I'} a_{n,k} e^{ik \cdot x}$$

can be obtained and compared to the outcome of FE and OE implementations in double precision arithmetic, respectively. In fact, an even simpler calculation can be performed in this case. Indeed, setting $Q_n = a_{n,n-1}$ and $P_n = d_{n,n+1}$ we have (see [24])

$$(22a) \quad Q_n = -2 \frac{(n-1)^n}{n!} - \sum_{l=2}^{n-1} \frac{(n-1)^{n-l}}{(n-l)!} Q_l$$

$$(22b) \quad P_n = - \sum_{l=0}^{n-1} \frac{(l+1)^{n-l}}{(n-l)!} P_l + \delta_{n,0}.$$

The computed values are displayed in Fig. 1, showing the detrimental effect of cancellations in formulas (21) and (14): in finite precision the values of Q_n and P_n lose approximately one digit of accuracy every time n increases by one and five, respectively.

Table 1. Significant digits in real part of $a_{n,1}$

n	FE	OE
2	16	16
4	15	15
6	15	15
8	14	14
10	13	14
12	12	14
14	10	12
16	7	11
18	5	6
20	2	5
22	0	2

Although suggestive of the overall behavior of the recursions (21) and (14) the example above does not provide us with an estimate of the loss of accuracy that can be expected on a *fixed* Fourier coefficient $a_k(\varepsilon)$ of the DNO

$$G(\varepsilon f) \xi(x) = \sum_{k \in \Gamma'} a_k(\varepsilon) e^{ik \cdot x}$$

when using the FE and OE approaches. For this, we have recorded in Table 1 the significant digits retained by FE and OE in the calculation of the Taylor coefficients $a_{n,1}$ of $a_1(\varepsilon)$, that is

$$a_1(\varepsilon) = \sum_{n=0}^{\infty} a_{n,1} \varepsilon^n$$

(the behavior for other coefficients $a_k(\varepsilon)$ is qualitatively similar, and it deteriorates with increasing wavenumber k). We see that even in this most favorable case of analytic, low frequency perturbations and Dirichlet data, there is a substantial loss of accuracy in the calculation of the coefficients $a_{n,1}$ as n increases: approximately one digit is lost every time the number of derivatives n increases by one beyond $n = 10$.

3 Analytic continuation: the method of transformed field expansions

From a theoretical standpoint, the cancellations in the FE and OE recursions conspire against a straightforward iterative estimation of the Taylor coefficients of the DNO. As we have shown [24], however, an alternative formulation that allows for such a strategy can be attained with a simple change of variables. Indeed, we have demonstrated that by *transforming* the perturbed domains onto the unperturbed geometry, a new set of recursive

formulas is obtained that is free of cancellations. These formulas were used in [24] to provide an alternative (simple) proof of analyticity of DNO and in [25] to introduce a new stable perturbative scheme for its evaluation, which we termed the method of “Transformed Field Expansions” (TFE). The results of [25] clearly establish the superior applicability and precision of TFE as it allows for accurate *high-order* calculations.

Still, all theoretical and numerical results to date are obviously limited to the domain of convergence of the perturbation series about a separable geometry. On the other hand, perturbative methods deliver the full Taylor series of the DNO which, as we know, suffices to determine the operators *throughout their domain of analyticity*. In this section we shall show, using a generalization of the TFE approach, that this domain of analyticity actually extends well beyond the disk of convergence. This, in turn, implies that classical mechanisms of analytic continuation may be incorporated into perturbative procedures thus enabling predictions for very large deformations of the basic domain. In Sect. 5 we demonstrate that this can be numerically realized, for instance, with the aid of Padé approximants.

To investigate the domain of analyticity of DNO we shall consider a fixed profile $f(x)$ and the operator

$$G(\delta f)$$

which we shall show is analytic for $\delta \in \mathbf{R}$ as long as $y = \delta f$ does not intersect the bottom boundary of the domain of definition. In particular, our results will imply that for a domain of depth h the operator is analytic in a complex neighborhood of the interval $[-h/\mu, h/\mu]$ where $\mu = |f|_{L^\infty}$ (and in all of \mathbf{R} if $h = \infty$).

For the sake of definiteness we shall assume that $h = 1$ and we shall consider a fixed $\delta_0 \in [-1/\mu, 1/\mu]$. Writing

$$f_0 = \delta_0 f, \quad \varepsilon = \delta - \delta_0,$$

for δ near δ_0 , we have

$$G(\delta f) = G(f_0 + \varepsilon f)$$

and our problem reduces to establishing analyticity in ε at $\varepsilon = 0$. For this, following [24], we introduce the change of variables

$$(23a) \quad x' = x$$

$$(23b) \quad y' = \frac{y - f_0(x) - \varepsilon f(x)}{1 + f_0(x) + \varepsilon f(x)},$$

which maps $S_{f_0+\varepsilon f}$ onto the strip S_0 . The change of variables (23) transforms v into

$$(24) \quad u(x', y', \varepsilon) = v(x', y' + (f_0 + \varepsilon f)(1 + y'), \varepsilon),$$

and (2) into

$$(25a) \quad \mathcal{L}'u = F(x', y', \varepsilon) \quad \text{in } S_0$$

$$(25b) \quad u(x', 0, \varepsilon) = \xi(x')$$

$$(25c) \quad \partial_{y'}u(x', -1, \varepsilon) = 0$$

$$(25d) \quad u(x' + \gamma, y', \varepsilon) = u(x', y', \varepsilon) \quad \text{for all } \gamma \in \Gamma.$$

The operator \mathcal{L}' and the function $F(x', y')$ are defined respectively as

$$(26) \quad \begin{aligned} \mathcal{L}'u \equiv & \operatorname{div}_{x'} \left[\nabla_{x'}u - \frac{(\nabla_{x'}f_0)(1+y')}{1+f_0} \partial_{y'}u \right] \\ & + \partial_{y'} \left[\frac{1}{(1+f_0)^2} \partial_{y'}u - \frac{(\nabla_{x'}f_0)(1+y')}{1+f_0} \cdot \nabla_{x'}u \right. \\ & \quad \left. + \frac{|\nabla_{x'}f_0|^2(1+y')^2}{(1+f_0)^2} \partial_{y'}u \right] \\ & + \frac{\nabla_{x'}f_0}{1+f_0} \cdot \nabla_{x'}u - \frac{|\nabla_{x'}f_0|^2(1+y')}{(1+f_0)^2} \partial_{y'}u, \end{aligned}$$

and

$$(27) \quad \begin{aligned} F(x', y', \varepsilon) \equiv & \operatorname{div}_{x'} \left[\left\{ \frac{(\nabla_{x'}f_0 + \varepsilon \nabla_{x'}f)(1+y')}{1+f_0 + \varepsilon f} \right. \right. \\ & \quad \left. \left. - \frac{(\nabla_{x'}f_0)(1+y')}{1+f_0} \right\} \partial_{y'}u \right] \\ & + \partial_{y'} \left[\left\{ -\frac{1}{(1+f_0 + \varepsilon f)^2} + \frac{1}{(1+f_0)^2} \right\} \partial_{y'}u \right. \\ & + \left\{ \frac{(\nabla_{x'}f_0 + \varepsilon \nabla_{x'}f)(1+y')}{1+f_0 + \varepsilon f} - \frac{(\nabla_{x'}f_0)(1+y')}{1+f_0} \right\} \cdot \nabla_{x'}u \\ & + \left. \left\{ -\frac{|\nabla_{x'}f_0 + \varepsilon \nabla_{x'}f|^2(1+y')^2}{(1+f_0 + \varepsilon f)^2} + \frac{|\nabla_{x'}f_0|^2(1+y')^2}{(1+f_0)^2} \right\} \partial_{y'}u \right] \\ & + \left\{ -\frac{\nabla_{x'}f_0 + \varepsilon \nabla_{x'}f}{1+f_0 + \varepsilon f} + \frac{\nabla_{x'}f_0}{1+f_0} \right\} \cdot \nabla_{x'}u \\ & + \left\{ \frac{|\nabla_{x'}f_0 + \varepsilon \nabla_{x'}f|^2(1+y')}{(1+f_0 + \varepsilon f)^2} - \frac{|\nabla_{x'}f_0|^2(1+y')}{(1+f_0)^2} \right\} \partial_{y'}u. \end{aligned}$$

In these new coordinates, and upon dropping the primes, the DNO becomes

$$(28) \quad G(f_0 + \varepsilon f) \xi = -(\nabla_x f_0 + \varepsilon \nabla_x f) \cdot \nabla_x u(x, 0, \varepsilon) \\ + \frac{1 + |\nabla_x f_0 + \varepsilon \nabla_x f|^2}{1 + f_0 + \varepsilon f} \partial_y u(x, 0, \varepsilon).$$

Note that, since $\nabla_x u(x, 0, \varepsilon) = \nabla_x \xi(x)$, to evaluate (28) it suffices to compute $\partial_y u(x, 0, \varepsilon)$. Thus, expanding

$$(29) \quad u(x, y, \varepsilon) = \sum_{n=0}^{\infty} u_n(x, y) \varepsilon^n,$$

we need only find

$$\partial_y u(x, 0, \varepsilon) = \sum_{n=0}^{\infty} \partial_y u_n(x, 0) \varepsilon^n.$$

The equations for u_n are

$$(30a) \quad \mathcal{L}u_n = (1 - \delta_{n,0})F_n(x, y) \quad \text{in } S_0 \\ (30b) \quad u_n(x, 0) = \delta_{n,0}\xi(x) \\ (30c) \quad \partial_y u_n(x, -1) = 0 \\ (30d) \quad u_n(x + \gamma, y) = u_n(x, y) \quad \text{for all } \gamma \in \Gamma,$$

where \mathcal{L} is given by (26) (with the primes omitted) and

$$(31) \quad F_n(x, y) = \operatorname{div}_x \left[F_n^{(1)}(x, y) \right] + \partial_y F_n^{(2)}(x, y) + F_n^{(3)}(x, y).$$

The functions $F_n^{(j)}$ are given by

$$(32a) \quad F_n^{(1)}(x, y) = \frac{1 + y}{1 + f_0} [(\nabla_x f_0)q + \nabla_x f] \sum_{j=0}^{n-1} q^j \partial_y u_{n-1-j},$$

$$\begin{aligned}
(32b) \quad F_n^{(2)}(x, y) &= -\frac{1}{(1+f_0)^2} \sum_{j=0}^{n-1} (j+2)q^{j+1} \partial_y u_{n-1-j} \\
&\quad + \frac{1+y}{1+f_0} [(\nabla_x f_0)q + \nabla_x f] \cdot \sum_{j=0}^{n-1} q^j \nabla_x u_{n-1-j} \\
&\quad - \frac{|\nabla_x f_0|^2 (1+y)^2}{(1+f_0)^2} \sum_{j=0}^{n-1} (j+2)q^{j+1} \partial_y u_{n-1-j} \\
&\quad - 2 \frac{(\nabla_x f_0) \cdot (\nabla_x f)(1+y)^2}{(1+f_0)^2} \sum_{j=0}^{n-1} (j+1)q^j \partial_y u_{n-1-j} \\
&\quad - \frac{|\nabla_x f|^2 (1+y)^2}{(1+f_0)^2} \sum_{j=0}^{n-2} (j+1)q^j \partial_y u_{n-2-j}
\end{aligned}$$

and

$$\begin{aligned}
(32c) \quad F_n^{(3)}(x, y) &= \frac{1}{1+f_0} [-(\nabla_x f_0)q - \nabla_x f] \cdot \sum_{j=0}^{n-1} q^j \nabla_x u_{n-1-j} \\
&\quad + \frac{|\nabla_x f_0|^2 (1+y)}{(1+f_0)^2} \sum_{j=0}^{n-1} (j+2)q^{j+1} \partial_y u_{n-1-j} \\
&\quad + 2 \frac{(\nabla_x f_0) \cdot (\nabla_x f)(1+y)}{(1+f_0)^2} \sum_{j=0}^{n-1} (j+1)q^j \partial_y u_{n-1-j} \\
&\quad + \frac{|\nabla_x f|^2 (1+y)}{(1+f_0)^2} \sum_{j=0}^{n-2} (j+1)q^j \partial_y u_{n-2-j}
\end{aligned}$$

where $q(x)$ is defined as

$$(33) \quad q(x) = -\frac{f(x)}{1+f_0(x)}.$$

Finally, the DNO can be formally expanded as

$$(34) \quad G(f_0 + \varepsilon f) \xi = \sum_{n=0}^{\infty} G_n(f_0, f) \xi \varepsilon^n.$$

where the n -th term in the expansion is

$$\begin{aligned}
 (35) \quad G_n(f_0, f) \xi &= -(\nabla_x f_0) \cdot (\nabla_x \xi) \delta_{n,0} - (\nabla_x f) \cdot (\nabla_x \xi) \delta_{n,1} \\
 &\quad + \frac{1 + |\nabla_x f_0|^2}{1 + f_0} \sum_{j=0}^n q^j \partial_y u_{n-j}(x, 0) \\
 &\quad + 2 \frac{\nabla_x f_0 \cdot \nabla_x f}{1 + f_0} \sum_{j=0}^{n-1} q^j \partial_y u_{n-1-j}(x, 0) \\
 &\quad \quad \quad + \frac{|\nabla_x f|^2}{1 + f_0} \sum_{j=0}^{n-2} q^j \partial_y u_{n-2-j}(x, 0).
 \end{aligned}$$

To recursively estimate the functions u_n we shall make repeated use of the inequality

$$(36) \quad \|fg\|_{H^s} \leq M |f|_{C^s} \|g\|_{H^s}$$

where $M = M(d, s)$ and which is valid for any $f \in C^s(P(\Gamma))$ and $g \in H^s(P(\Gamma) \times [-1, 0])$ where $P(\Gamma)$ is the basic periodicity cell associated with the lattice Γ . Our main result is:

Theorem 1 *Given an integer $s \geq 0$, if $f_0, f \in C^{s+2}(P(\Gamma))$ and $\xi \in H^{s+3/2}(P(\Gamma))$, there exist constants $C_0 = C_0(d, s, |f_0|_{C^{s+2}})$, $K_0 = K_0(d, s, |f_0|_{C^{s+2}})$, and a unique solution (29) of Eqn. (25) satisfying*

$$(37) \quad \|u_n\|_{H^{s+2}(P(\Gamma) \times [-1, 0])} \leq K_0 \|\xi\|_{H^{s+3/2}(P(\Gamma))} B^n$$

for any $B > \max\{3 |f|_{C^{s+2}} K_0 C_0, 2M(d, s) |q|_{C^{s+1}}\}$.

From this the analyticity of DNO follows immediately by combining (37) and (35). Indeed, we have

Theorem 2 *For an integer $s \geq 0$, if $f_0, f \in C^{s+2}(P(\Gamma))$ then the series (34) converges strongly as an operator from $H^{s+3/2}(P(\Gamma))$ to $H^{s+1/2}(P(\Gamma))$. More precisely, there exists a constant*

$$K_0^* = K_0^*(d, s, |f_0|_{C^{s+2}})$$

such that

$$(38) \quad \|G_n(f_0, f) \xi\|_{H^{s+1/2}(P(\Gamma))} \leq K_0^* \|\xi\|_{H^{s+3/2}(P(\Gamma))} B^n,$$

for any $B > \max\{3 |f|_{C^{s+2}} K_0 C_0, 2M(d, s) |q|_{C^{s+1}}\}$.

Note that, using (33), we have

$$\max\{3|f|_{C^{s+2}} K_0 C_0, 2M(d, s) |q|_{C^{s+1}}\} \leq C_0^*(d, s, |f_0|_{C^{s+2}}) |f|_{C^{s+2}}$$

so that, as expected, the radius of convergence of the series (29) and (34) depend linearly on the size of the perturbation f .

As we said, to derive (38) it suffices to establish Thm. 1. For this we shall show that the Sobolev norms of the functions u_n can be recursively controlled from (30) by appealing to classical elliptic estimates. In our case, these estimates correspond to the periodic analogue of Theorem 8.13 in [11], which we record here for the sake of completeness.

Lemma 1 *For an integer $s \geq 0$ there exists a constant*

$$K_0 = K_0(d, s, |f_0|_{C^{s+2}})$$

such that for any $\xi \in H^{s+3/2}(P(\Gamma))$ and $g^{(j)} \in H^{s+1}(P(\Gamma) \times [-1, 0])$, the solution $w(x, y)$ of

$$\mathcal{L}w(x, y) = \operatorname{div}_x [g^{(1)}(x, y)] + \partial_y g^{(2)}(x, y) + g^{(3)}(x, y) \quad \text{in } S_0$$

$$w(x, 0) = \xi(x)$$

$$\partial_y w(x, -1) = 0$$

$$w(x + \gamma, y) = w(x, y) \quad \text{for all } \gamma \in \Gamma$$

satisfies

$$\|w\|_{H^{s+2}(P(\Gamma) \times [-1, 0])} \leq K_0 \left[\|\xi\|_{H^{s+3/2}(P(\Gamma))} + \sum_{j=1}^3 \|g^{(j)}\|_{H^{s+1}(P(\Gamma) \times [-1, 0])} \right].$$

The recursive estimation of the functions u_n demand that we obtain bounds on the right hand sides of (30) at each step of the inductive procedure. With this in mind we next establish

Lemma 2 *Let $s \geq 0$ be an integer and let $f_0, f \in C^{s+2}(P(\Gamma))$. Assume*

$$(40) \quad \|u_n\|_{H^{s+2}(P(\Gamma) \times [-1, 0])} \leq K_1 B^n$$

for $n < N$ and constants $K_1, B > 0$. Then if

$$B > \max\{|f|_{C^{s+2}}, 2M(d, s) |q|_{C^{s+1}}\}$$

there exists a constant $C_0 = C_0(d, s, |f_0|_{C^{s+2}})$ such that the functions $F_N^{(j)}$ in (32) satisfy

$$(41) \quad \left\| F_N^{(j)} \right\|_{H^{s+1}(P(\Gamma) \times [-1, 0])} \leq K_1 |f|_{C^{s+2}} C_0 B^{N-1}.$$

Proof. For the sake of brevity we shall only consider the term $F_N^{(3)}$; $F_N^{(1)}$ and $F_N^{(2)}$ can be similarly handled. From (32c) and (36) we have

$$\begin{aligned} \left\| F_N^{(3)} \right\|_{H^{s+1}} &\leq M^2 \left| \frac{1}{1 + f_0} \right|_{C^{s+1}} \left[M |f|_{C^{s+1}} \left| \frac{\nabla_x f_0}{1 + f_0} \right|_{C^{s+1}} + |f|_{C^{s+2}} \right] \\ &\quad \times \sum_{j=0}^{N-1} M^j |q|_{C^{s+1}}^j \left\| \nabla_x u_{N-1-j} \right\|_{H^{s+1}} \\ &\quad + M^2 |f|_{C^{s+1}} \left| \frac{\nabla_x f_0 \cdot \nabla_x f_0}{(1 + f_0)^3} \right|_{C^{s+1}} \\ &\quad \times \sum_{j=0}^{N-1} (j + 2) M^j |q|_{C^{s+1}}^j 2 \left\| \partial_y u_{N-1-j} \right\|_{H^{s+1}} \\ &\quad + 2M^2 |f|_{C^{s+2}} \left| \frac{\nabla_x f_0}{(1 + f_0)^2} \right|_{C^{s+1}} \\ &\quad \times \sum_{j=0}^{N-1} (j + 1) M^j |q|_{C^{s+1}}^j 2 \left\| \partial_y u_{N-1-j} \right\|_{H^{s+1}} \\ &\quad + M^3 |f|_{C^{s+2}}^2 \left| \frac{1}{1 + f_0} \right|_{C^{s+1}}^2 \\ &\quad \times \sum_{j=0}^{N-2} (j + 1) M^j |q|_{C^{s+1}}^j 2 \left\| \partial_y u_{N-2-j} \right\|_{H^{s+1}} \end{aligned}$$

where we have used

$$\left\| (1 + y)g \right\|_{H^{s+1}(P(\Gamma) \times [-1, 0])} \leq 2 \left\| g \right\|_{H^{s+1}(P(\Gamma) \times [-1, 0])}$$

which holds for any $g \in H^{s+1}(P(\Gamma) \times [-1, 0])$. Then, using (40), we get

$$\begin{aligned} \left\| F_N^{(3)} \right\|_{H^{s+1}} &\leq K_1 |f|_{C^{s+2}} C B^{N-1} \sum_{j=0}^{N-1} \left(\frac{M |q|_{C^{s+1}}}{B} \right)^j \\ &\quad + K_1 |f|_{C^{s+2}} C B^{N-1} \sum_{j=0}^{N-1} (j+2) \left(\frac{M |q|_{C^{s+1}}}{B} \right)^j \\ &\quad + K_1 |f|_{C^{s+2}} C B^{N-1} \sum_{j=0}^{N-1} (j+1) \left(\frac{M |q|_{C^{s+1}}}{B} \right)^j \\ &\quad + K_1 |f|_{C^{s+2}} C \left(\frac{|f|_{C^{s+2}}}{B} \right) B^{N-1} \sum_{j=0}^{N-2} (j+1) \left(\frac{M |q|_{C^{s+1}}}{B} \right)^j \end{aligned}$$

where $C = C(d, s, |f_0|_{C^{s+2}})$. Finally, if $B > |f|_{C^{s+2}}$, the estimate (41) follows provided that $B > 2M |q|_{C^{s+1}}$.

Proof. (Theorem 1) The proof of the estimate (37) proceeds inductively. The case $n = 0$ follows directly from Lemma 1 ($g^{(j)} = 0$). Now assume that (37) holds for all $n < N$. Again an application of Lemma 1 implies that

$$\|u_N\|_{H^{s+2}(P(\Gamma) \times [-1, 0])} \leq K_0 \sum_{j=1}^3 \left\| F_N^{(j)} \right\|_{H^{s+1}(P(\Gamma) \times [-1, 0])}.$$

Thus, from Lemma 2 (letting $K_1 = K_0 \|\xi\|_{s+3/2}$) we obtain

$$\|u_N\|_{H^{s+2}(P(\Gamma) \times [-1, 0])} \leq K_0 3 \left\{ K_0 \|\xi\|_{H^{s+3/2}(P(\Gamma))} \right\} C_0 |f|_{C^{s+2}} B^{N-1},$$

and (37) holds provided that $3K_0 C_0 |f|_{C^{s+2}} < B$.

4 Joint analyticity

As we said (see Sect. 2.2), the basic recursions underlying the OE and FE methods involve high order derivatives of the perturbation profile f and therefore demand a suitable interpretation if f is not smooth. This remark was actually at the core of our observation that these recurrences are rather unstable [24]. In fact, the very validity of the OE and FE formulas (in the strong sense in which they were proposed) becomes questionable for a general profile of finite regularity. On the other hand, the formulas would be completely justified if the potential u could be shown to be holomorphic in (x, y, ε) up to and beyond the boundary $y = f_0(x) + \varepsilon f(x)$, for in this case all differentiations leading to the recurrence would be amply substantiated.

In this section we show that such a result can be derived for analytic perturbations f with a suitable modification of the arguments in Sect. 3. As stated in the introduction, an analogous result in the context of scattering applications was previously derived in [3]. There, the analyticity of the scattered fields was established with a subtle use of potential theoretic and complex analytic techniques that avoided any reference to the corresponding recursions. In particular, for instance, the extension to three dimensional space was not immediate, due to the different nature of the singularities of the corresponding surface potentials [2]. In contrast, our approach here is based once again on the direct estimation of the (transformed) recursions (30), and it therefore easily extends to any number of dimensions and, in fact, to a variety of other physical scenarios (including the scattering applications of [3, 2]).

For simplicity of presentation we establish the analyticity result in the setting of perturbations from a flat domain ($f_0 = 0$); the extension to general basic (analytic) geometries is straightforward. Of course, to establish the joint analyticity of the potential u in (x, y, ε) up to and beyond the boundary $y = \varepsilon f(x)$, we must certainly require that both the perturbation f itself and the Dirichlet data ξ be spatially analytic. In particular, we must have that

$$(42a) \quad \left| \frac{\partial_x^k}{|k|!} \xi \right|_{C^2} \leq C_\xi \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2} \quad \forall k$$

$$(42b) \quad \left| \frac{\partial_x^k}{|k|!} f \right|_{C^2} \leq C_f \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2} \quad \forall k$$

and some constants $C_\xi, C_f, A \in \mathbf{R}$. Here we use “multi-index” notation where, for $l = (l_1, \dots, l_{d-1})$

$$\begin{aligned} \partial_x^l &= \partial_{x_1}^{l_1} \dots \partial_{x_{d-1}}^{l_{d-1}} \\ l! &= l_1! \dots l_{d-1}! \\ |l| &= l_1 + \dots + l_{d-1} \end{aligned}$$

and if $r = (r_1, \dots, r_{d-1})$ then $r \leq l$ if and only if $r_j \leq l_j$ for $j = 1 \dots d-1$. For such data, our main result is

Theorem 3 *If f and ξ satisfy (42) then the solution*

$$u(x, y, \varepsilon) = \sum_{n=0}^{\infty} u_n(x, y) \varepsilon^n$$

of Eqn. (25) ($f_0 = 0$) satisfies

$$(43) \quad \left\| \frac{\partial_x^k \partial_y^l}{(|k| + l)!} u_n \right\|_{H^2} \leq K_2 C_\xi B^n \frac{D^l}{(l + 1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2} \quad \forall k, l, n$$

for any $B > K_3 C_f$, $D > C(1 + A)$, where C , K_2 and K_3 are constants depending only on d .

Remark 1 Note that if (43) holds then, since

$$\frac{1}{k!l!} \leq \frac{d^{|k|+l}}{(|k|+l)!},$$

we have

$$\left\| \frac{\partial_x^k \partial_y^l \partial_\varepsilon^n}{k! l! n!} u(\cdot, 0) \right\|_{H^2} \leq K_2 C_\xi B^n \frac{(dD)^l}{(l+1)^2} \prod_{j=1}^{d-1} \frac{(dA)^{k_j}}{(k_j+1)^2}$$

so that the function $u(x, y, \varepsilon)$ is indeed jointly analytic in (x, y, ε) . Furthermore, from equation (35) it is clear that joint analyticity of $u(x, y, \varepsilon)$ leads directly to that of DNO.

We shall prove Theorem 3 by induction in l . Thus we must first establish (43) for $l = 0$ which we accomplish, for each k , with an inductive procedure in the order n . More precisely we first show that

Lemma 3 *If f and ξ satisfy (42) then, there exist constants $K_2 = K_2(d)$, $K_4 = K_4(d)$ such that*

$$(44) \quad \left\| \frac{\partial_x^k}{|k|!} u_n \right\|_{H^2} \leq K_2 C_\xi B^n \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j+1)^2} \quad \forall k, n$$

and any $B > K_4 C_f$.

To prove Lemma 3 we need

Lemma 4 *Let f satisfy (42) and assume*

$$\left\| \frac{\partial_x^k}{|k|!} u_n \right\|_{H^2} \leq K_2 C_\xi B^n \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j+1)^2} \quad \forall k,$$

for all $n < N$, and for some constants $K_2, B > 0$. Then if $B > 2C_f S$ (with S as in (64)) there exists a constant $K_5 = K_5(d)$ such that the functions $F_N^{(j)}$ in (32) satisfy

$$(45) \quad \left\| \frac{\partial_x^k}{|k|!} F_N^{(j)} \right\|_{H^1} \leq K_2 K_5 C_\xi C_f B^{N-1} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j+1)^2} \quad \forall k.$$

Proof. As before, for the sake of brevity, we shall only consider the term $F_n^{(3)}$; the other terms can be dealt with in the same manner. From (32c) we have

$$\begin{aligned}
\left\| \frac{\partial_x^k}{|k|!} F_N^{(3)} \right\|_{H^1} &\leq M \sum_{l=0}^{N-1} \sum_{r \leq k} \left\| \frac{\partial_x^r}{|r|!} [(\nabla_x f)(-f)^l] \right\|_{C^1} \\
&\quad \times \left\| \frac{\partial_x^{k-r}}{|k-r|!} \nabla_x u_{N-1-l} \right\|_{H^1} \frac{k! |r|! |k-r|!}{|k|! r! (k-r)!} \\
&\quad + 2M \sum_{l=0}^{N-2} (l+1) \sum_{r \leq k} \left\| \frac{\partial_x^r}{|r|!} [|\nabla_x f|^2 (-f)^l] \right\|_{C^1} \\
&\quad \times \left\| \frac{\partial_x^{k-r}}{|k-r|!} \partial_y u_{N-2-l} \right\|_{H^1} \frac{k! |r|! |k-r|!}{|k|! r! (k-r)!} \\
&\leq M \sum_{l=0}^{N-1} \sum_{r \leq k} \left\| \frac{\partial_x^r}{|r|!} [(\nabla_x f)(-f)^l] \right\|_{C^1} \\
&\quad \times \left\| \frac{\partial_x^{k-r}}{|k-r|!} \nabla_x u_{N-1-l} \right\|_{H^1} \\
&\quad + 2M \sum_{l=0}^{N-2} (l+1) \sum_{r \leq k} \left\| \frac{\partial_x^r}{|r|!} [|\nabla_x f|^2 (-f)^l] \right\|_{C^1} \\
&\quad \times \left\| \frac{\partial_x^{k-r}}{|k-r|!} \partial_y u_{N-2-l} \right\|_{H^1}
\end{aligned} \tag{46}$$

where we have used the inequality

$$\frac{k!}{r!(k-r)!} \leq \frac{|k|!}{|r|! |k-r|!}. \tag{47}$$

On the other hand, from Lemma 7 we have

$$\begin{aligned}
\left\| \frac{\partial_x^r}{|r|!} [(\nabla_x f)(-f)^l] \right\|_{C^1} &= \left\| (-1) \frac{\partial_x^r}{|r|!} \nabla_x \left[\frac{(-f)^{l+1}}{l+1} \right] \right\|_{C^1} \\
&\leq \left\| \frac{\partial_x^r}{|r|!} \left[\frac{(-f)^{l+1}}{l+1} \right] \right\|_{C^2} \\
&\leq \frac{C_f^{l+1} S^{l-1}}{l+1} \prod_{j=1}^{d-1} \frac{A^{r_j}}{(r_j+1)^2}
\end{aligned} \tag{48}$$

and, again using (47),

(49)

$$\begin{aligned}
\left\| \frac{\partial_x^r}{|r|!} \left[|\nabla_x f|^2 (-f)^l \right] \right\|_{C^1} &= \left\| (-1) \frac{\partial_x^r}{|r|!} \left[(\nabla_x f) \cdot \nabla_x \left[\frac{(-f)^{l+1}}{l+1} \right] \right] \right\|_{C^1} \\
&\leq \sum_{s \leq r} \left\| \frac{\partial_x^s}{|s|!} f \right\|_{C^2} \left\| \frac{\partial_x^{r-s}}{|r-s|!} \frac{(-f)^{l+1}}{l+1} \right\|_{C^2} \frac{r! |s|! |r-s|!}{|r|! s! (r-s)!} \\
&\leq \sum_{s \leq r} C_f \prod_{j=1}^{d-1} \frac{A^{s_j}}{(s_j+1)^2} \frac{C_f^{l+1}}{l+1} S^l \prod_{j=1}^{d-1} \frac{A^{r_j-s_j}}{(r_j-s_j+1)^2} \\
&\leq \frac{C_f^{l+2}}{l+1} S^{l+1} \prod_{j=1}^{d-1} \frac{A^{r_j}}{(r_j+1)^2}.
\end{aligned}$$

Combining (46), (48), and (49) we get

$$\begin{aligned}
\left\| \frac{\partial_x^k}{|k|!} F_N^{(3)} \right\|_{H^1} &\leq M \sum_{l=0}^{N-1} \sum_{r \leq k} \frac{C_f^{l+1} S^l}{l+1} \prod_{j=1}^{d-1} \frac{A^{r_j}}{(r_j+1)^2} K_2 C_\xi B^{N-1-l} \\
&\quad \times \prod_{j=1}^{d-1} \frac{A^{k_j-r_j}}{(k_j-r_j+1)^2} \\
&\quad + 2M \sum_{l=0}^{N-2} \sum_{r \leq k} C_f^{l+2} S^{l+1} \prod_{j=1}^{d-1} \frac{A^{r_j}}{(r_j+1)^2} K_2 C_\xi B^{N-2-l} \\
&\quad \times \prod_{j=1}^{d-1} \frac{A^{k_j-r_j}}{(k_j-r_j+1)^2} \\
&\leq M K_2 C_\xi B^{N-1} C_f \left[\sum_{l=0}^{N-1} \left(\frac{C_f S}{B} \right)^l \right] \left(1 + 2 \left(\frac{C_f S}{B} \right) \right) \\
&\quad \times \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j+1)^2} \left[\sum_{r_j=0}^{k_j} \frac{(k_j+1)^2}{(r_j+1)^2 (k_j-r_j+1)^2} \right] \\
&\leq M K_2 C_\xi B^{N-1} C_f \left[\sum_{l=0}^{N-1} \left(\frac{C_f S}{B} \right)^l \right] \\
&\quad \times \left(1 + 2 \left(\frac{C_f S}{B} \right) \right) S \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j+1)^2}
\end{aligned}$$

so that (45) follows provided $(C_f S)/B < 1/2$.

Proof. (Lemma 3) The proof proceeds inductively in n ; notice that since the u_n satisfy (30) (with $f_0 = 0$), the functions $[\partial_x^k/k!]u_n$ satisfy

$$(50a) \quad \Delta \frac{\partial_x^k}{|k|!} u_n = (1 - \delta_{n,0}) \frac{\partial_x^k}{|k|!} F_n \quad \text{in } S_0$$

$$(50b) \quad \frac{\partial_x^k}{|k|!} u_n(x, 0) = \delta_{n,0} \frac{\partial_x^k}{|k|!} \xi(x)$$

$$(50c) \quad \partial_y \frac{\partial_x^k}{|k|!} u_n(x, -1) = 0$$

$$(50d) \quad \frac{\partial_x^k}{|k|!} u_0(x + \gamma, y) = \frac{\partial_x^k}{|k|!} u_0(x, y) \quad \text{for all } \gamma \in \Gamma.$$

In the case $n = 0$, Lemma 1 and the analyticity of ξ imply

$$\left\| \frac{\partial_x^k}{|k|!} u_0 \right\|_{H^2} \leq K_0 \left\| \frac{\partial_x^k}{|k|!} \xi \right\|_{H^{3/2}} \leq K_2 C_\xi \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}$$

for all indices $k \geq 0$. Now suppose that

$$\left\| \frac{\partial_x^k}{|k|!} u_n \right\|_{H^2} \leq K_2 C_\xi B^n \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}$$

for all $n < N$ and all indices $k \geq 0$. Using Lemma 1 we can estimate

$$\left\| \frac{\partial_x^k}{|k|!} u_N \right\|_{H^2} \leq K_0 \sum_{j=1}^3 \left\| \frac{\partial_x^k}{|k|!} F_N^{(j)} \right\|_{H^1}.$$

Finally, using Lemma 4 we obtain

$$\left\| \frac{\partial_x^k}{|k|!} u_N \right\|_{H^2} \leq 3K_0 K_2 K_5 C_\xi C_f B^{N-1} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2},$$

and the proof is complete provided that $K_4 = \max\{2S, 3K_0 K_5\}$.

Lemma 3 establishes (43) for $l = 0$. To enable the inductive step for $l > 0$ we will need the following two results.

Lemma 5 *If ξ satisfies (42) then the solution $w(x, y)$ of*

$$(51a) \quad \Delta w(x, y) = 0 \quad \text{in } S_0$$

$$(51b) \quad w(x, 0) = \xi(x)$$

$$(51c) \quad \partial_y w(x, -1) = 0$$

$$(51d) \quad w(x + \gamma, y) = w(x, y) \quad \text{for all } \gamma \in \Gamma$$

satisfies

$$(52) \quad \left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} w \right\|_{H^2} \leq K_2 C_\xi \frac{D^L}{(L + 1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2} \quad \forall k, L$$

provided that $D > C(1 + A)$ where $C = C(d)$ is a constant.

Proof. To simplify the notation we shall denote by $C(d)$ a generic constant depending only on dimension. From Lemma 3 we have the estimate in the case $L = 0$. Proceeding by induction, assume that the estimate holds for all $l < L$, then

$$\begin{aligned} \left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} w \right\|_{H^2} &\leq \left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} w \right\|_{H^1} + \left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} \nabla_x w \right\|_{H^1} \\ &\quad + \left\| \frac{\partial_x^k \partial_y^{L+1}}{(|k| + L)!} w \right\|_{H^1} \\ &\leq \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} w \right\|_{H^2} + \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} \nabla_x w \right\|_{H^2} \\ &\quad + C(d) \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} \nabla_x w \right\|_{H^2}, \end{aligned}$$

the last term coming from the fact that w solves Laplace's equation. By the inductive assumption

$$\left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} w \right\|_{H^2} \leq K_2 C_\xi \frac{D^{L-1}}{L^2} C(d)(1 + A) \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}$$

and the proof is complete as long as $D \geq C(1 + A)$.

Lemma 6 *Let f satisfy (42). Assume*

$$(53) \quad \left\| \frac{\partial_x^k \partial_y^l}{(|k| + l)!} u_n \right\|_{H^2} \leq K_2 C_\xi B^n \frac{D^l}{(l + 1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}$$

for all indices $n, k \geq 0$, when $l < L$, and for all $k \geq 0$ and $n < N$ when $l = L$. Then there exists a constant $K_6 = K_6(d)$ such that the function F_N in (31) satisfies

$$(54) \quad \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} F_N \right\|_{H^1} \leq K_2 K_6 C_\xi C_f B^{N-1} \frac{D^L}{(L + 1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2} \quad \forall k$$

provided that $B > 2C_f S$.

Proof. We first note that from (31)

$$(55) \quad \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k|+L)!} F_N \right\|_{H^1} \leq \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k|+L)!} \operatorname{div}_x [F_N^{(1)}] \right\|_{H^1} + \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k|+L)!} \partial_y F_N^{(2)} \right\|_{H^1} + \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k|+L)!} F_N^{(3)} \right\|_{H^1}.$$

Once again, in the interests of brevity, we shall establish the bound (54) for the second term in (55) only; the other terms can be handled in a similar fashion. Moreover, since

$$\begin{aligned} \partial_y F_N^{(2)} = \partial_y \left[- \sum_{m=0}^{N-1} (m+2)(-f)^{m+1} \partial_y u_{N-1-m} \right. \\ \left. + (1+y) \nabla_x f \cdot \sum_{m=0}^{N-1} (-f)^m \nabla_x u_{N-1-m} \right. \\ \left. - |\nabla_x f|^2 (1+y)^2 \sum_{m=0}^{N-2} (m+1)(-f)^m \partial_y u_{N-2-m} \right] \end{aligned}$$

(c.f. (32b) ($f_0 = 0$)) we shall only estimate the last term, as the others can be dealt with more simply. We begin with

$$\begin{aligned} R &\equiv \left\| \frac{\partial_x^k \partial_y^L}{(|k|+L)!} \left[|\nabla_x f|^2 (1+y)^2 \sum_{m=0}^{N-2} (m+1)(-f)^m \partial_y u_{N-2-m} \right] \right\|_{H^1} \\ &\leq M \sum_{m=0}^{N-2} \sum_{k \leq r} (m+1) \left\| \frac{\partial_x^r}{|r|!} \left[|\nabla_x f|^2 (-f)^m \right] \right\|_{C^1} \\ &\quad \times \left\| \frac{\partial_x^{k-r} \partial_y^L}{(|k-r|+L)!} \left[(1+y)^2 \partial_y u_{N-2-m} \right] \right\|_{H^1} \frac{k! |r|! (|k-r|+L)!}{r! (k-r)! (|k|+L)!} \\ &\leq M \sum_{m=0}^{N-2} \sum_{k \leq r} C_f^{m+2} S^{m+1} \prod_{j=1}^{d-1} \frac{A^r}{(r_j+1)^2} \\ &\quad \times \left\| \frac{\partial_x^{k-r} \partial_y^L}{(|k-r|+L)!} \left[(1+y)^2 \partial_y u_{N-2-m} \right] \right\|_{H^1} \end{aligned}$$

where we have used (49) and

$$\frac{k! |r|! (|k-r|+L)!}{r! (k-r)! (|k|+L)!} \leq 1.$$

Next, since

$$\begin{aligned} \partial_y^L [(1+y)^2 \partial_y u_{N-2-m}] &= (1+y)^2 \partial_y^{L+1} u_{N-2-m} \\ &\quad + 2L(1+y) \partial_y^L u_{N-2-m} \\ &\quad + L(L-1) \partial_y^{L-1} u_{N-2-m} \end{aligned}$$

we can estimate

$$\begin{aligned} R &\leq M \sum_{m=0}^{N-2} \sum_{k \leq r} C_f^{m+2} S^{m+1} \prod_{j=1}^{d-1} \frac{A^{r_j}}{(r_j+1)^2} C(d) \\ &\quad \times \left\{ \left\| \frac{\partial_x^{k-r} \partial_y^L}{(|k-r|+L)!} u_{N-2-m} \right\|_{H^2} \right. \\ &\quad + L \left\| \frac{\partial_x^{k-r} \partial_y^{L-1}}{(|k-r|+L)!} u_{N-2-m} \right\|_{H^2} \\ &\quad \left. + L^2 \left\| \frac{\partial_x^{k-r} \partial_y^{L-2}}{(|k-r|+L)!} u_{N-2-m} \right\|_{H^2} \right\} \end{aligned}$$

so that, using (53), we obtain

$$\begin{aligned} R &\leq MC(d) C_f K_2 C_\xi B^{N-1} \left(\frac{C_f S}{B} \right)^{N-2} \sum_{m=0}^{N-2} \left(\frac{C_f S}{B} \right)^m \\ &\quad \times \sum_{k \leq r} \prod_{j=1}^{d-1} \frac{A^{r_j}}{(r_j+1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j-r_j}}{(k_j-r_j+1)^2} \\ &\quad \left(\frac{D^L}{(L+1)^2} + \frac{L}{|k-r|+L} \frac{D^{L-1}}{L^2} \right. \\ &\quad \left. + \frac{L^2}{(|k-r|+L)(|k-r|+L-1)} \frac{D^{L-2}}{(L-1)^2} \right) \\ &\leq MC(d) C_f K_2 C_\xi S B^{N-1} \frac{D^L}{(L+1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j+1)^2} \end{aligned}$$

and (54) follows provided that $K_6 \geq MC(d)S$.

Proof. (Theorem 3) Once again we work inductively. We begin with an induction on l . For $l = 0$ and any $k, n \geq 0$ we use Lemma 3. Now we assume

$$\left\| \frac{\partial_x^k \partial_y^l}{(|k|+l)!} u_n \right\|_{H^2} \leq K_2 C_\xi B^n \frac{D^l}{(l+1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j+1)^2}$$

for all $l < L$ and any $k, n \geq 0$, and seek to prove

$$(56) \quad \left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} u_n \right\|_{H^2} \leq K_2 C_\xi B^n \frac{D^L}{(L+1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}$$

for any $k, n \geq 0$. We accomplish this with another induction, this time on n . Lemma 5 gives (56) in the case $n = 0$. We next assume

$$\left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} u_n \right\|_{H^2} \leq K_2 C_\xi B^n \frac{D^L}{(L+1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}$$

for all $n < N$ and seek to establish

$$\left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} u_N \right\|_{H^2} \leq K_2 C_\xi B^N \frac{D^L}{(L+1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}.$$

We proceed with

$$\begin{aligned} \left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} u_N \right\|_{H^2} &\leq \left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} u_N \right\|_{H^1} + \left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} \nabla_x u_N \right\|_{H^1} \\ &\quad + \left\| \frac{\partial_x^k \partial_y^{L+1}}{(|k| + L)!} u_N \right\|_{H^1} \\ &\leq \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} u_N \right\|_{H^2} + \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} \nabla_x u_N \right\|_{H^2} \\ &\quad + \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} \Delta_x u_N \right\|_{H^1} + \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} F_N \right\|_{H^1} \\ &\leq \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} u_N \right\|_{H^2} + \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} \nabla_x u_N \right\|_{H^2} \\ &\quad + C(d) \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} \nabla_x u_N \right\|_{H^2} + \left\| \frac{\partial_x^k \partial_y^{L-1}}{(|k| + L)!} F_N \right\|_{H^1} \end{aligned}$$

where C is a generic function of dimension and we have used the fact that u_N solves (30a). Using Lemma 6 we get

$$\begin{aligned} \left\| \frac{\partial_x^k \partial_y^L}{(|k| + L)!} u_N \right\|_{H^2} &\leq K_2 C_\xi [1 + C(d)A] B^N \frac{D^{L-1}}{L^2} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2} \\ &\quad + K_2 C_\xi [K_6 C_f] B^{N-1} \frac{D^L}{(L+1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2} \end{aligned}$$

and the desired estimate holds provided that $D > C(1+A)$ and $B > K_6 C_f$.

5 Numerical implementation and results

As we anticipated, the relevance of the analytic continuation results established in previous sections goes beyond the theoretical. Indeed, Theorem 2 guarantees the existence of a complex neighborhood of the interval $[-1/|f|_{L^\infty}, 1/|f|_{L^\infty}]$ in the ε complex plane where DNO is holomorphic. On the other hand, the formulas (10), (21), (35) ($f_0 = 0$) produce the full Taylor series of the operators at $\varepsilon = 0$ and these, of course, completely determine the DNO throughout their domain of analyticity. Thus, our theoretical results suggest a means to enhance the performance of perturbative approaches, namely by “numerical analytic continuation” of the power series of the DNO. In this section we present numerical results that illustrate how this can, in fact, be attained with classical Padé approximation [1]. These examples show that, overall, substantial gains in performance can be achieved regardless of the particular perturbative implementation (OE, FE or TFE). Moreover, they further show that the improved stability properties of TFE [25], which allow for very high-order calculations, can result in significantly more accurate results over those produced by the classical OE and FE realizations.

5.1 Numerical implementation

The implementation of OE is based upon the evaluation of Eqn. (21) (or its analogue in finite depth). The periodic boundary conditions in the x variable and the conspicuous appearance of Fourier multipliers in the formula naturally suggest a Fourier spectral method. In this scheme the unknowns are represented by Fourier series of a fixed order $N_x/2$ (with N_x collocation points) and all nonlinearities are evaluated using fast convolutions via the FFT algorithm. These calculations are partially de-aliased: a product of two series of size $N_x/2$ is computed exactly (in the form of a series of size N_x) and *a posteriori* truncated back to size $N_x/2$.

The FE approximation, on the other hand, is constructed from the recurrence (14) (or its analogue in finite depth) and the representation (10). Once again a Fourier basis is very natural and we thus use a Fourier spectral approach with fast, partially de-aliased convolutions.

The implementation of the TFE approximation is somewhat different from that of the OE and FE methods. Indeed, both the OE and FE approaches rely on the homogeneity of the differential equation (11a) to express the solutions *in closed form* as linear combinations of suitable basis functions (exponentials in this case, cf. (13), (16)). In contrast, the “source terms” in (30) preclude the use of a standard basis for the exact representation of solutions, which we therefore approximate numerically. As we shall demonstrate, the consequent increase in computational cost is compensated by a

substantial increase in accuracy that can, in fact, allow for computations beyond the reach of the OE and FE algorithms (see also [25]).

For the numerical solution of (30) we have chosen a spectral Fourier/Chebyshev-tau method which posits an approximate solution of the form

$$\tilde{u}_n(x, y) = \sum_{k \in \Gamma', |k| < N_x/2} \sum_{l=0}^{N_y} \hat{u}_n(k, l) e^{ik \cdot x} T_l(2y + 1)$$

where $T_l(z)$ is the l -th Chebyshev polynomial. The resulting set of equations can be efficiently solved via the use of fast Fourier and Chebyshev transforms in conjunction with the fast elliptic solve outlined in [13, §10]. Finally, the DNO is approximated from this representation through Eqn. (35).

All three methods deliver spectral approximations of DNO in the form

$$\begin{aligned} G_N^{\text{approx}}(\varepsilon f) \xi &= \sum_{n=0}^N \sum_{k \in \Gamma'} a_{n,k} e^{ik \cdot x} \varepsilon^n \\ &= \sum_{k \in \Gamma'} S_k^N(\varepsilon) e^{ik \cdot x} \end{aligned}$$

for ε small, where $S_k^N(\varepsilon)$ is a truncated Taylor series of the k -th Fourier coefficient $S_k(\varepsilon)$. On the other hand, our results ensure the possibility of extending the functions $S_k(\varepsilon)$, and therefore the DNO, beyond the disk of convergence of their power series about $\varepsilon = 0$. For the numerical realization of such analytic continuations, we shall resort here to Padé approximation [1]. We recall that the $[P, Q]$ Padé approximant to a series

$$(57) \quad S(\varepsilon) = \sum_{n=0}^{\infty} a_n \varepsilon^n$$

is the unique rational function of order P over Q which coincides with $S(\varepsilon)$ to order $P + Q + 1$. In the experiments below we use diagonal or paradiagonal Padé sequences. As is well-known, Padé approximants have some remarkable properties of approximation of (a large subclass of) analytic functions from their Taylor series (57) for points far outside their radii of convergence, see e.g. [1]. They can be calculated by first solving a set of linear equations for the denominator coefficients, and then using simple formulas to compute the numerator coefficients.

5.2 Numerical results

In this section we present numerical results for representative surface profiles in two and three dimensions. Our first set of experiments are designed

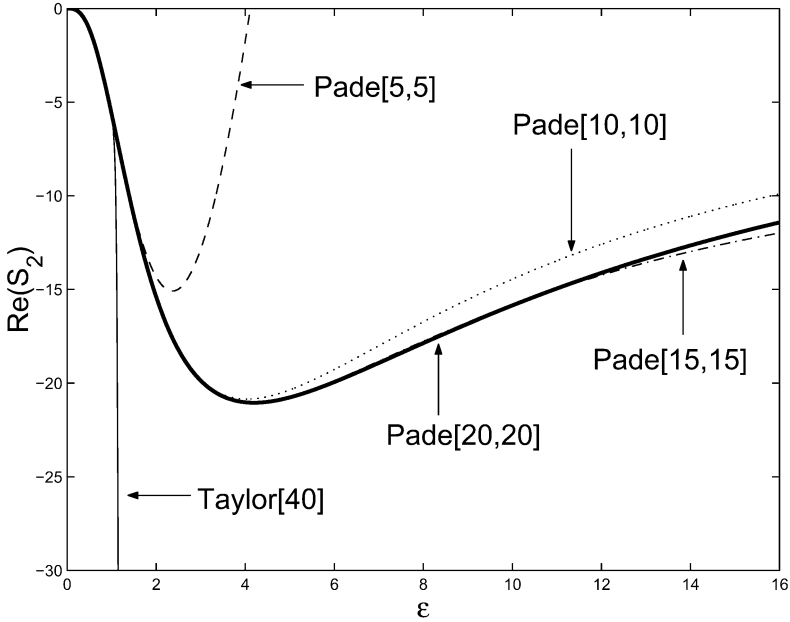


Fig. 2. Plot of approximations to $\text{Re}(S_2(\varepsilon))$ for $f(x_1) = \cos(x_1)$ and $\xi(x_1) = \cos(x_1)$: Taylor series of order 40, and Padé approximations of order [5,5], [10,10], [15,15], and [20,20]

to demonstrate the exceptional performance of Padé approximation in the numerical analytic continuation of power series. For this, we consider the evaluation of the Taylor series (7) of the DNO corresponding to the profile $y = f(x_1) = \cos(x_1)$ applied to Dirichlet data $\xi(x_1) = \cos(x_1)$ in two dimensions. The results in Fig. 2 were obtained with a TFE implementation with $N_x = 256$ and $N_y = 64$. The outcome of such computations consists of the coefficients $a_{n,k}$ of the Taylor expansion of each Fourier mode $S_k(\varepsilon)$ in the spectral representation of the function (7). Figure 2 contains plots of the Taylor series and various Padé approximants to the second mode $S_2(\varepsilon)$, which clearly show the convergence of the diagonal Padé sequence; the effect on other modes is similar. Moreover, the figure also shows the very significant extension of the domain of convergence of a perturbative algorithm when used in combination with Padé approximation.

In a second set of experiments we compare the performance of each of the three implementations (OE, FE, TFE), with and without Padé approximation, on some model two and three-dimensional profiles. To allow for very significant perturbations without topological complications we have chosen to experiment on domains of depth $h = 10$, that is

$$S_f = \{(x, y) \in \mathbf{R}^{d-1} \times \mathbf{R} \mid -10 < y < f(x)\}.$$

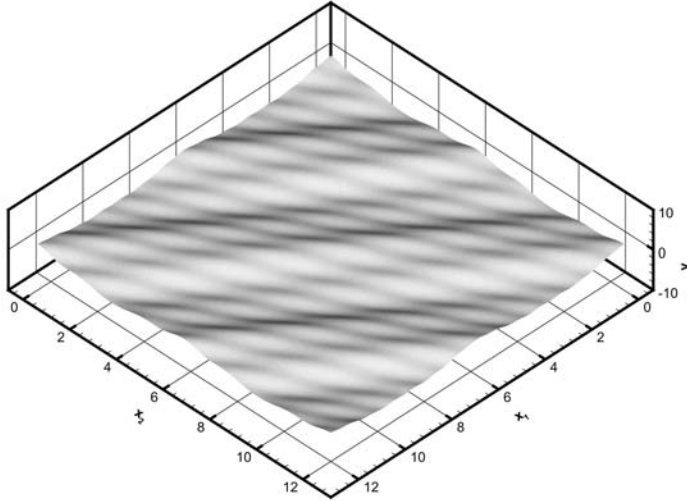


Fig. 3. Plot of g_o , the “rough ocean” profile

We consider a smooth sinusoidal profile

$$(58a) \quad f_s(x_1) = \cos(x_1)$$

and a Lipschitz profile

$$(58b) \quad f_L(x_1) = \begin{cases} -\frac{2}{\pi}x_1 + 1 & 0 \leq x_1 < \pi \\ \frac{2}{\pi}x_1 - 3 & \pi \leq x_1 < 2\pi \end{cases}$$

in two dimensions, and a rather generic profile

$$(58c) \quad g_o(x_1, x_2) = \cos(x_1 + x_2) + \frac{1}{3} \cos(2x_1 + 3x_2) + \frac{1}{9} \cos(7x_1 + 4x_2).$$

reminiscent of a “rough ocean,” in three dimensions (see Fig. 3). To test the convergence of the algorithms in each case we consider exact solutions to (2) of the form

$$(59) \quad v_k(x, y) = \cosh(|k|(y + 1)) \cos(k \cdot x).$$

For these, we obviously have

$$(60) \quad G(\varepsilon f)(v_k(x, \varepsilon f(x))) = \nabla v_k|_{y=\varepsilon f} \cdot (-\varepsilon \nabla_x f, 1)^T$$

for any function f . Then, for the outcome of a numerical simulation, the defect in this relation (e.g. in the discrete L^2 norm) can be used as an error estimate.

Figures 4 and 5 display results with $N_x = 256$ and $N_y = 64$ for the profile (58a). The figures correspond to two different values of ε , one inside the disk of convergence of the Taylor series ($\varepsilon = 1.0$) and one outside ($\varepsilon = 2.0$). We see then that Padé approximation substantially enhances the performance of *each* algorithm not only by enlarging the domain of applicability (Fig. 5) but also by accelerating the rate of convergence of the Taylor series whenever it has a finite sum (Fig. 4). Moreover, the effect of ill-conditioning in the OE and FE approaches is quite evident here as these results sharply deviate from those given by the TFE method beyond a critical order ($n = 10$ for OE and $n = 20$ for FE). Indeed, the continued reduction in the error displayed by the TFE implementation as n increases demonstrates that the OE and FE results are genuinely corrupted beyond these critical values. This corruption can be attributed solely to ill-conditioning as the number of Fourier modes retained in the calculation ($N_x/2 = 128$) is sufficient to guarantee the absence of substantial aliasing errors.

Similar comments apply to Figs. 6 and 7 corresponding to the sawtooth profile (58b) again performed with $N_x = 256$ and $N_y = 64$. For computational purposes the Fourier series representation of the profile must, of course, be truncated. Here, for illustration, we have chosen to approximate (58b) with a Fourier series of order 20. In this case, and in contrast with the sinusoidal profile, the resolution of our computations is not sufficient to preclude potentially significant aliasing errors (e.g. the n -th power of the truncated profile will contain modes of order $20n$ so that aliasing occurs if $20n > 128$). However, computations with larger values of N_x do not yield improved results for the OE and FE implementations which again implies that their observed divergence from the TFE results is due to ill-conditioning.

Finally we present in Figs. 8 and 9 results for the profile (58c) performed with $N_{x_1} = 64$, $N_{x_2} = 64$, and $N_y = 64$. Here, the onset of divergence of the OE and FE methods appears at a relatively low order ($n = 5$) in spite of the smoothness of the profile, hinting to the possible effects of aliasing errors. In fact, Figs. 10 and 11, which display the results of calculations with $N_{x_1} = N_{x_2} = 128$, confirm this conjecture: further de-aliasing results in divergence at a higher order ($n = 10$). In other words, this example demonstrates a further limitation of the OE and FE algorithms, which compute quantities with larger high-frequency content than those produced by TFE. As a result, Padé approximation has little effect for OE and FE in these calculations since the higher order derivatives are not accurately computed. In contrast,

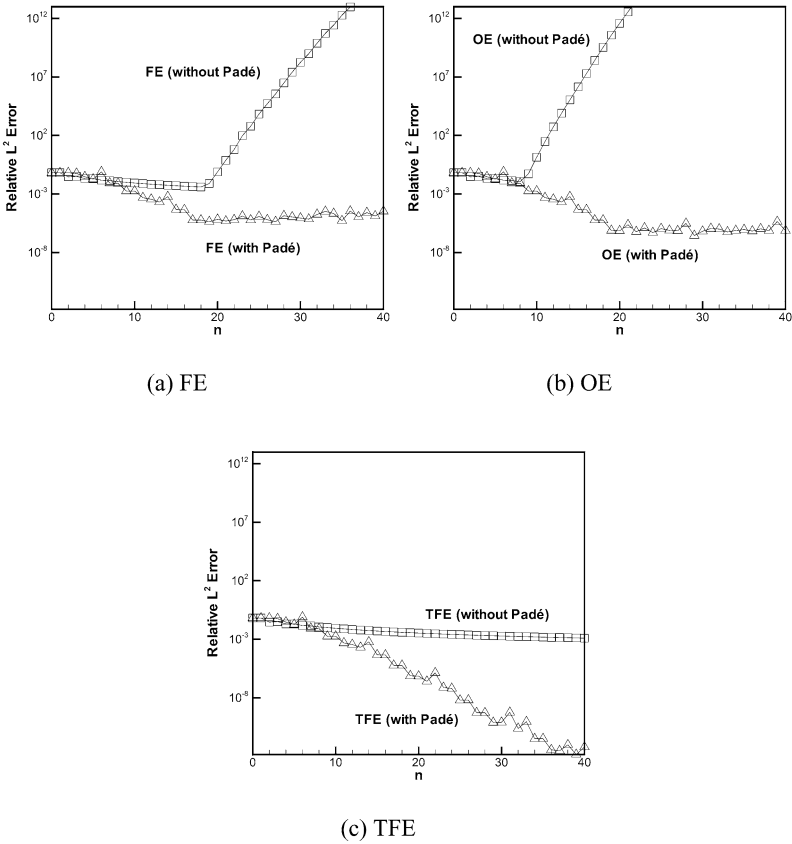


Fig. 4. Convergence of FE, OE, TFE with smooth profile in 2D ($\epsilon = 1.0$)

a substantial improvement is observed when Padé approximation is used in conjunction with the TFE approach.

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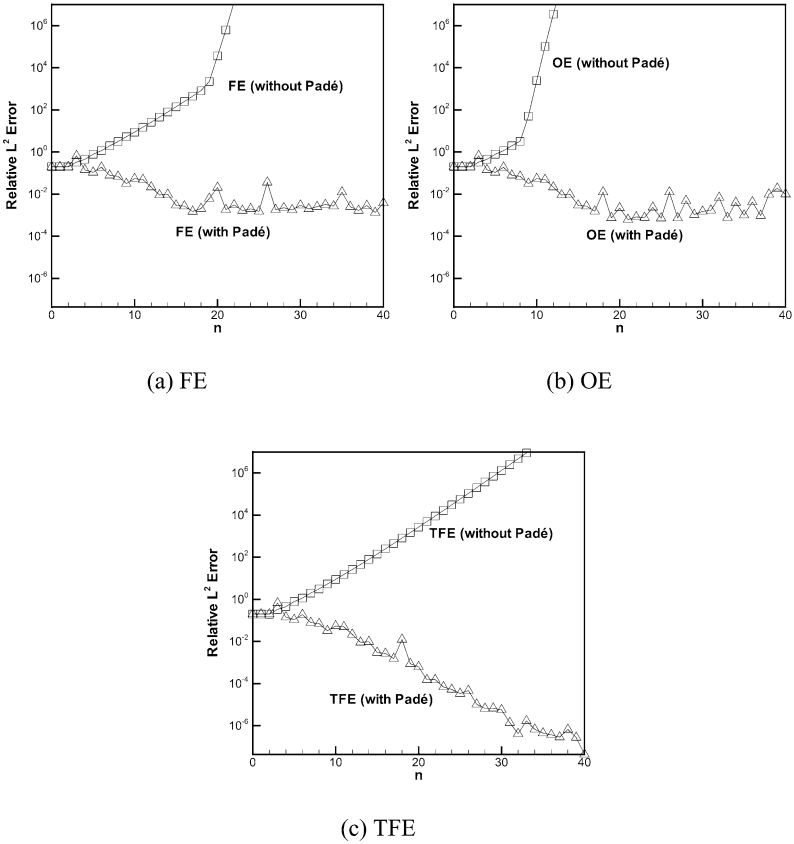


Fig. 5. Convergence of FE, OE, TFE with smooth profile in 2D ($\epsilon = 2.0$)

A Estimates on products of analytic functions

Lemma 7 *Given analytic functions $g, h \in C^\omega(P(\Gamma))$ which satisfy*

$$(61) \quad \left| \frac{\partial_x^k}{|k|!} g \right|_{C^2} \leq C_g \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}$$

$$(62) \quad \left| \frac{\partial_x^k}{|k|!} h \right|_{C^2} \leq C_h \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}$$

we have

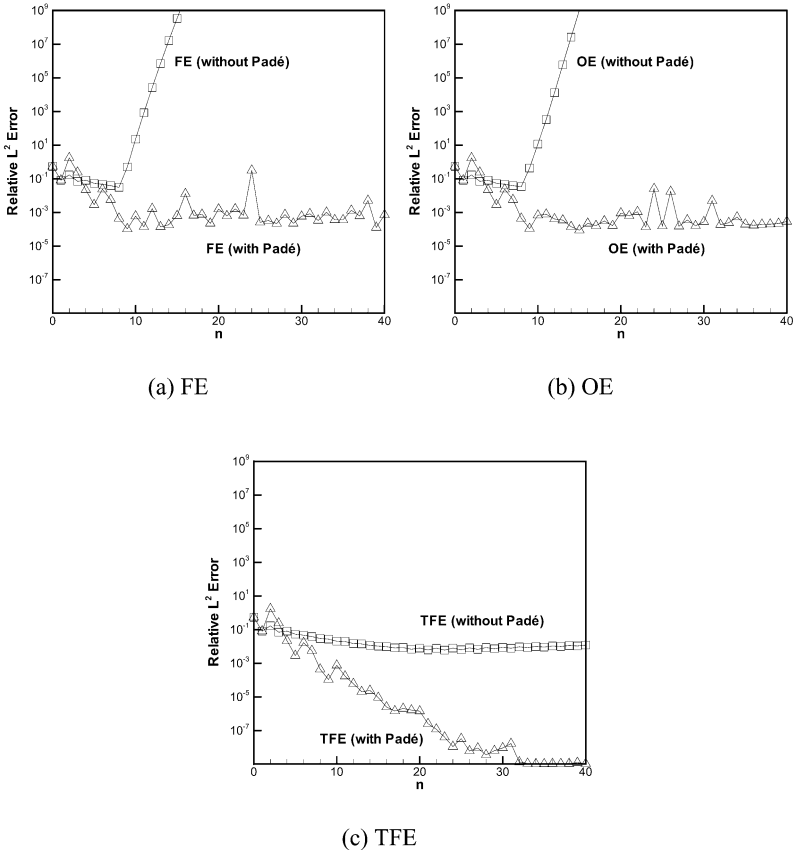


Fig. 6. Convergence of FE, OE, TFE with Lipschitz profile in 2D ($\varepsilon = 1.3$)

$$(63a) \quad \left| \frac{\partial_x^k}{|k|!} (gh) \right|_{C^2} \leq C_g C_h S \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}$$

$$(63b) \quad \left| \frac{\partial_x^k}{|k|!} (g^l) \right|_{C^2} \leq C_g^l S^{l-1} \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}$$

$$(63c) \quad \left| \frac{\partial_x^k}{|k|!} (g^l h) \right|_{C^2} \leq C_g^l C_h S^l \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j + 1)^2}$$

where

$$(64) \quad S = S(d) = \left(\sum_{p=0}^{\infty} \frac{8}{(p+1)^2} \right)^{d-1} = \left(\frac{4\pi^2}{3} \right)^{d-1}.$$

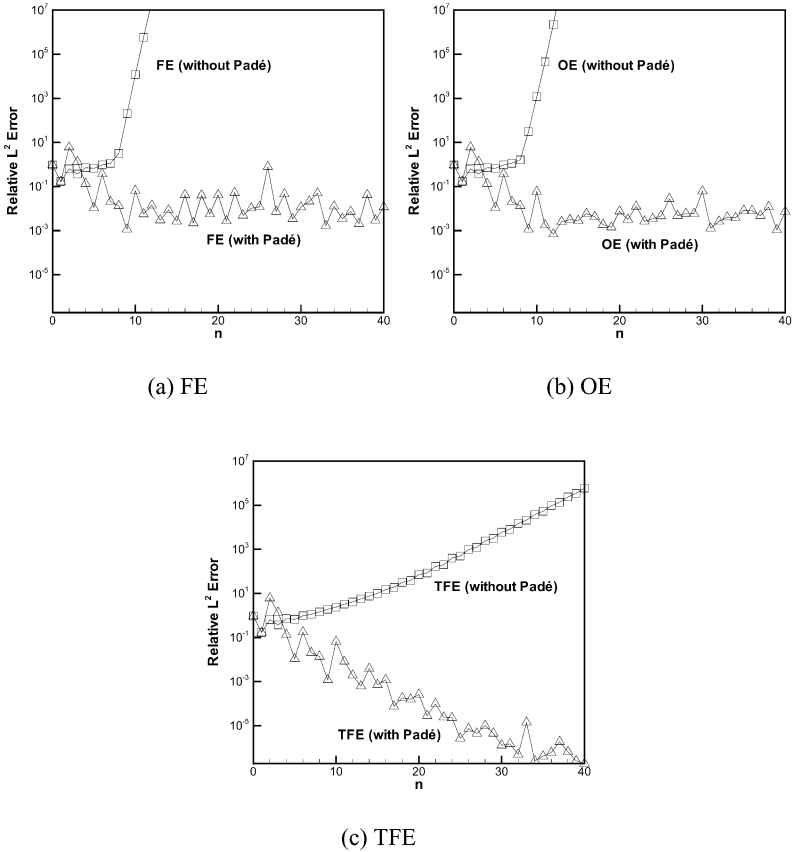


Fig. 7. Convergence of FE, OE, TFE with Lipschitz profile in 2D ($\varepsilon = 2.0$)

Proof. It suffices to establish (63a). For this we compute

$$\begin{aligned}
 \left| \frac{\partial_x^k}{|k|!} (gh) \right|_{C^2} &\leq \sum_{0 \leq m \leq k} 2 \frac{|\partial_x^m g|_{C^2}}{|m|!} \frac{|\partial_x^{k-m} h|_{C^2}}{|k-m|!} \left(\frac{|m|! |k-m|! k!}{m!(k-m)! |k|!} \right) \\
 &\leq 2C_g C_h \sum_{0 \leq m \leq k} \prod_{j=1}^{d-1} \frac{A^{m_j}}{(m_j+1)^2} \prod_{j=1}^{d-1} \frac{A^{k_j-m_j}}{(k_j-m_j+1)^2} \\
 &\leq 2C_g C_h \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j+1)^2} \sum_{m_j=0}^{k_j} \frac{(k_j+1)^2}{(m_j+1)^2 (k_j-m_j+1)^2} \\
 &\leq 2SC_g C_h \prod_{j=1}^{d-1} \frac{A^{k_j}}{(k_j+1)^2}
 \end{aligned}$$

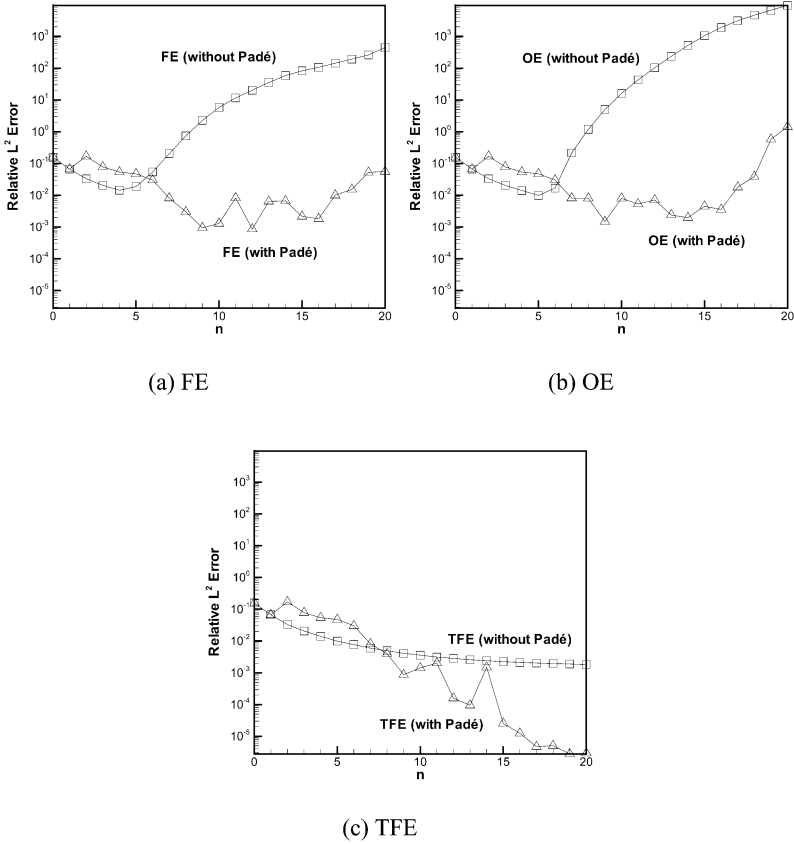


Fig. 8. Convergence of FE, OE, TFE with ocean profile in 3D ($\varepsilon = 0.3$)

which holds by (47) and since

$$|fg|_{C^2} = \sum_{k=0}^2 \left| \partial_x^k (fg) \right|_{L^\infty} \leq 2 |g|_{C^2} |f|_{C^2}$$

and (for integers p and q)

$$\begin{aligned} & \sum_{p=0}^q \frac{(q+1)^2}{(p+1)^2 (q-p+1)^2} \\ &= \sum_{p=0}^{[q/2]} \frac{(q+1)^2}{(p+1)^2 (q-p+1)^2} + \sum_{p=[q/2]}^q \frac{(q+1)^2}{(p+1)^2 (q-p+1)^2} \end{aligned}$$

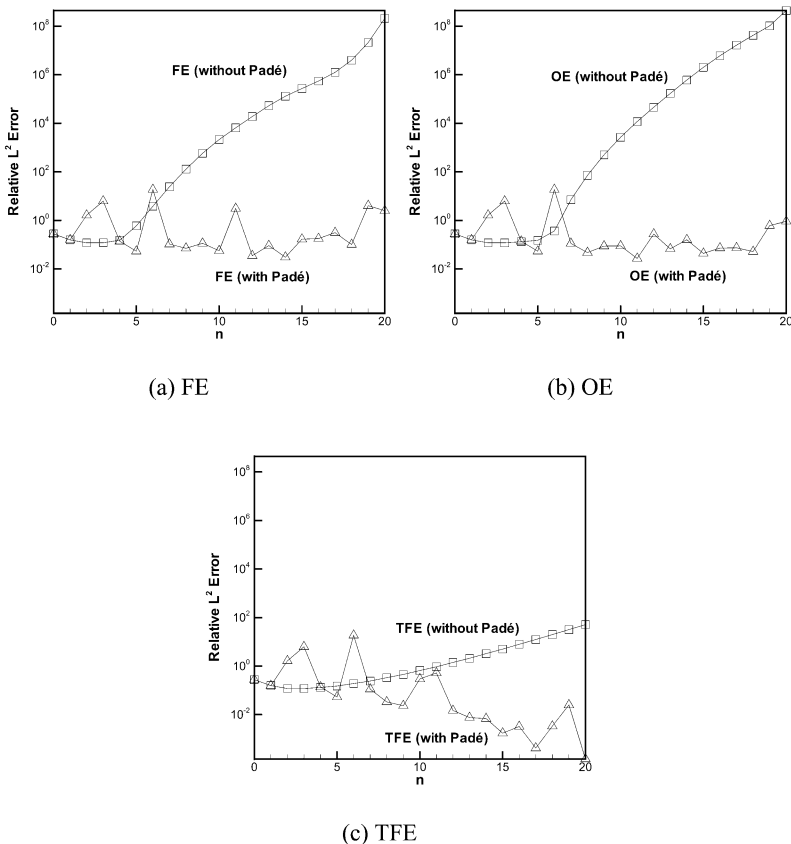


Fig. 9. Convergence of FE, OE, TFE with ocean profile in 3D ($\varepsilon = 0.5$)

$$\begin{aligned}
 &\leq \sum_{p=0}^{\lfloor q/2 \rfloor} \frac{(q+1)^2}{(p+1)^2(q-q/2+1)^2} + \sum_{p=\lfloor q/2 \rfloor}^q \frac{(q+1)^2}{(q/2+1)^2(q-p+1)^2} \\
 &\leq \sum_{p=0}^{\lfloor q/2 \rfloor} \frac{4(q+1)^2}{(p+1)^2(q+2)^2} + \sum_{p=\lfloor q/2 \rfloor}^q \frac{4(q+1)^2}{(q+2)^2(q-p+1)^2} \\
 &\leq 4 \sum_{p=0}^{\lfloor q/2 \rfloor} \frac{1}{(p+1)^2} + 4 \sum_{p=\lfloor q/2 \rfloor}^q \frac{1}{(q-p+1)^2} \\
 &\leq 8 \sum_{p=0}^{\lfloor q/2 \rfloor + 1} \frac{1}{(p+1)^2} \leq 8 \sum_{p=0}^{\infty} \frac{1}{(p+1)^2}.
 \end{aligned}$$

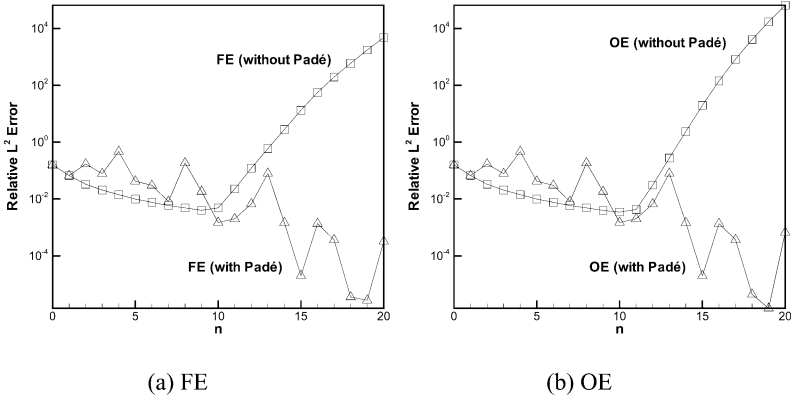


Fig. 10. Convergence of FE and OE with ocean profile in 3D ($\varepsilon = 0.3$) with higher precision

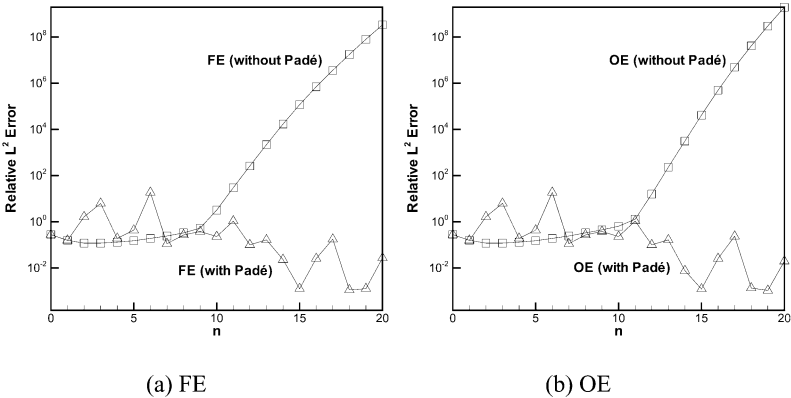


Fig. 11. Convergence of FE and OE with ocean profile in 3D ($\varepsilon = 0.5$) with higher precision

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