High–Order Perturbation of Surfaces (HOPS) Short Course: Boundary Value Problems

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Abstract In this lecture we introduce two classical High–Order Perturbation of Surfaces (HOPS) computational schemes in the simplified context of elliptic boundary value problems inspired by models in water waves. For the problem of computing Dirichlet–Neumann Operators (DNOs) for Laplace's equation, we outline Bruno & Reitich's method of Field Expansions (FE) and then describe Milder and Craig & Sulem's method of Operator Expansions (OE). We further show how these algorithms can be extended to three dimensions and finite depth, and describe how Padé approximation can be used as a method of numerical analytic continuation to realize enhanced performance and applicability through a series of numerical experiments.

1 Introduction

The Calculus in general, and Partial Differential Equations (PDEs) in particular have long been recognized as the most powerful and successful mathematical modeling tool for engineering and science, and the study of surface water waves is no exception. With the advent of the modern computer in the 1950s, the possibility of numerical simulation of PDEs at last became a practical reality. The last 50–60 years has seen an explosion in the development and implementation of algorithms for this purpose which are rapid, robust, and highly accurate. Among the myriad choices are:

1. Finite Difference methods (e.g., [Str04, MM05, LeV07, Tho95]),
2. Finite Element methods (Continuous and Discontinuous) (e.g., [Joh87, KS99, Bra01, HW08]),

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3. High–Order Spectral (Element) methods (e.g., [GO77, CHQZ88, For96, Boy01, DFM02, HGG07]),
4. Boundary Integral/Element methods (e.g., [CK98, Kre99]).

The class of High–Order Perturbation of Surfaces (HOPS) methods we describe here are a High–Order Spectral method which is particularly well–suited for PDEs posed on *piecewise homogeneous domains*. Such "layered media" problems abound in the sciences, e.g., in

- free–surface fluid mechanics (e.g., the water wave problem),
- acoustic waves in piecewise constant density media,
- electromagnetic waves interacting with grating structures,
- elastic waves in sediment layers.

For such problems these HOPS methods can be:

- *highly accurate* (error decaying *exponentially* as the number of degrees of freedom increases),
- *rapid* (an order of magnitude fewer unknowns as compared with volumetric formulations),
- *robust* (delivering accurate results for rather rough/large interface shapes).

However, these HOPS schemes are *not* competitive for problems with inhomogeneous domains and/or "extreme" geometries.

In this lecture we discuss two classical HOPS methods for the solution of such interfacial problems: Bruno & Reitich's Field Expansions (FE) method [BR92, BR93a, BR93b, BR93c, BR94, BR96, BR98, BR01], and Milder and Craig & Sulem's Operator Expansions (OE) method [Mil91a, Mil91b, MS91, MS92, CS93, Mil96b, Mil96a]. In a future lecture we discuss a stabilized version of the FE method (the Transformed Field Expansions–TFE–method) due to the author and Reitich [NR01a, NR01b, NR03]. In addition to specifying the details of these two algorithms (FE and OE) for a particular problem which arises in the study of water waves, we also want to illustrate the accuracy, efficiency, speed, and ease of implementation of HOPS schemes.

The rest of the lecture is organized as follows. In § 2 we recall the classical water wave problem and how the Dirichlet–Neumann Operator (DNO) arises as a fundamental object of study. In § 3 and § 4 we give the details of the Field Expansions and Operator Expansions methods, respectively, as applied to the problem of simulating the DNO. In § 5 we present results of numerical simulations realized with a simple MATLAB implementation of these recursions. In § 6 we discuss generalization of these algorithms to three dimensions and finite depth. We close with a presentation of the Padé approximation approach in § 7 to analytic continuation for these problems, and the extremely beneficial effect this methodology can have on these HOPS methods.

2 Water Waves and the Dirichlet–Neumann Operator

To fix on a problem we consider a classical water wave problem [Lam93] which is to model the evolution of the free surface of a deep, two–dimensional, ideal fluid under the influence of gravity. The widely accepted model [Lam93] is

$$\begin{aligned}
&\Delta \varphi = 0 && y < \eta(x,t),\\
&\partial_y \varphi \to 0 && y \to -\infty,\\
&\partial_t \eta + \partial_x \eta (\partial_x \varphi) = \partial_y \varphi, && y = \eta(x,t),\\
&\partial_t \varphi + (1/2) \nabla \varphi \cdot \nabla \varphi + \tilde{g} \eta = 0 && y = \eta(x,t).
\end{aligned}$$

In these $\varphi(x,y,t)$ is the velocity potential ($\mathbf{u} = \nabla \varphi$), $\eta(x,t)$ is the air–water interface, and $\tilde{g}$ is the gravitational constant.

At the center of this problem is the solution of the elliptic Boundary Value Problem (BVP)

$$\begin{aligned}
&\Delta v = 0 && y < g(x),\\
&\partial_y v \to 0 && y \to -\infty,\\
&v = \xi && y = g(x).
\end{aligned}$$

In particular, upon solving this problem, the *Dirichlet–Neumann Operator (DNO)*

$$G(g)[\xi] := [\partial_y v - (\partial_x g) \partial_x v]_{y=g(x)},$$

allows one to recast the water wave problem as [Zak68, CS93]

$$\begin{aligned}
\partial_t \eta &= G(\eta)\xi,\\
\partial_t \xi &= -\tilde{g}\eta - A(\eta) B(\eta, \xi),
\end{aligned}$$

where

$$\begin{aligned}
A &= \left[2\left(1 + (\partial_x \eta)^2\right)\right]^{-1},\\
B &= (\partial_x \xi)^2 - (G(\eta)\xi)^2 - 2(\partial_x \eta)(\partial_x \xi)(G(\eta)\xi).
\end{aligned}$$

For many problems of practical interest it suffices to consider the classical periodic boundary conditions, e.g.,

$$v(x+L,y) = v(x,y), \quad g(x+L) = g(x), \quad L = 2\pi,$$

which permits us to express functions in terms of their Fourier Series

$$g(x) = \sum_{p=-\infty}^{\infty} \hat{g}_p e^{ipx}, \quad \hat{g}_p = \frac{1}{2\pi} \int_0^{2\pi} g(s) e^{-ips} \, ds.$$

Thus, from here we focus on the BVP

$$
\begin{aligned}
&\Delta v = 0 && y < g(x), && \text{(1a)}\\
&\partial_y v \to 0 && y \to -\infty, && \text{(1b)}\\
&v = \xi && y = g(x), && \text{(1c)}\\
&v(x+2\pi, y) = v(x,y), && && \text{(1d)}
\end{aligned}
$$

and the DNO it generates.

3 The Method of Field Expansions

Our first HOPS approach for approximating DNOs solves the BVP, (1), directly. Its origins can be found in the work of Rayleigh [Ray07] and Rice [Ric51]. The first *high–order* implementation is due to Bruno & Reitich [BR93a, BR93b, BR93c] and was originally denoted the "method of Variation of Boundaries." To prevent confusion with subsequent methods it was later renamed the method of Field Expansions (FE). The "key" to the method is the realization that interior to the domain (i.e., $y < -|g|_\infty$) the solution of Laplace's equation by separation of variables is

$$
v(x,y) = \sum_{p=-\infty}^{\infty} a_p e^{|p|y} e^{ipx}. \tag{2}
$$

This HOPS approach uses the fact that, for a sufficiently smooth boundary perturbation $g(x) = \varepsilon f(x)$, the field, $v = v(x,y;\varepsilon)$, depends *analytically* upon ε.

Assume that the interface is shaped by $g(x) = \varepsilon f(x)$ where $f \sim \mathscr{O}(1)$ and, initially, $\varepsilon \ll 1$. We will be able to show *a posteriori* that v depends *analytically* upon ε so that

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

Inserting this expansion into the governing equations, (1), and equating at orders $\mathscr{O}(\varepsilon^n)$ yields

$$
\begin{aligned}
&\Delta v_n = 0 && y < 0, && \text{(3a)}\\
&\partial_y v_n \to 0 && y \to -\infty, && \text{(3b)}\\
&v_n = Q_n && y = 0, && \text{(3c)}\\
&v_n(x+2\pi, y) = v_n(x,y). && && \text{(3d)}
\end{aligned}
$$

The crucial term is the boundary inhomogeneity

$$
Q_n(x) = \delta_{n,0}\xi(x) - \sum_{m=0}^{n-1} F_{n-m}(x)\ \partial_y^{n-m} v_m(x,0),
$$

where $F_m(x) := \frac{f^m(x)}{m!}$ and $\delta_{n,m}$ is the Kronecker delta. This form comes from the expansion

$$v(x,\varepsilon f;\varepsilon) = \sum_{n=0}^{\infty} v_n(x,\varepsilon f)\varepsilon^n = \sum_{n=0}^{\infty} \varepsilon^n \sum_{m=0}^{n} F_{n-m}(x)\ \partial_y^{n-m} v_m(x,0).$$

Bounded, periodic solutions of Laplace's equation can be expressed as

$$v_n(x,y) = \sum_{p=-\infty}^{\infty} a_{n,p} e^{|p|y} e^{ipx}. \tag{4}$$

Inserting this form into the surface boundary condition, (3c), delivers

$$\sum_{p=-\infty}^{\infty} a_{n,p} e^{ipx} = \sum_{p=-\infty}^{\infty} \hat{Q}_{n,p} e^{ipx},$$

where, since

$$e^{|p|\varepsilon f} = \sum_{m=0}^{\infty} \varepsilon^m F_m \left|p\right|^m,$$

we have

$$Q_n(x) = \delta_{n,0} \sum_{p=-\infty}^{\infty} \hat{\xi}_p e^{ipx} - \sum_{m=0}^{n-1} F_{n-m}(x) \sum_{p=-\infty}^{\infty} \left|p\right|^{n-m} a_{m,p} e^{ipx}.$$

Summarizing, we have the *FE Recursions*

$$a_{n,p} = \delta_{n,0}\hat{\xi}_p - \sum_{m=0}^{n-1} \sum_{q=-\infty}^{\infty} \hat{F}_{n-m,p-q} \left|q\right|^{n-m} a_{m,q}. \tag{5}$$

The FE recursions deliver the solution everywhere *well inside* the problem domain. However, two questions immediately arise: Is the expansion

$$v(x,y) = \sum_{p=-\infty}^{\infty} a_p e^{|p|y} e^{ipx}$$

valid at the *boundary*? Is this expansion valid *near* the boundary? For rigorous answers to these questions we refer to Bruno & Reitich's first contribution [BR92], the work of the author and Reitich [NR01a, NR01b, NR03], and the third lecture in this series.

Assuming for the moment that there is some validity at the boundary, recall that we wish to compute the Neumann data

$$\nu(x) = \left[\partial_y v - (\partial_x g)\partial_x v\right]_{y=g(x)}.$$

Expanding in ε

$$\sum_{n=0}^{\infty} \nu_n(x)\varepsilon^n = \sum_{n=0}^{\infty} \left[\partial_y v_n(x,\varepsilon f) - \varepsilon(\partial_x f)\partial_x v_n(x,\varepsilon f)\right]\varepsilon^n,$$

and equating at order $\mathscr{O}(\varepsilon^n)$ gives

$$\nu_n(x) = \sum_{m=0}^{n} F_{n-m}\partial_y^{n+1-m} v_m(x,0) - \sum_{m=0}^{n-1} (\partial_x f)F_{n-1-m}\partial_x\partial_y^{n-1-m} v_m(x,0).$$

At each wavenumber we have

$$\hat{\nu}_{n,p} = \sum_{m=0}^{n}\sum_{q=-\infty}^{\infty} \hat{F}_{n-m,p-q}\,|q|^{n+1-m}\,a_{m,q} \\ - \sum_{m=0}^{n-1}\sum_{q=-\infty}^{\infty} \hat{F}'_{n-1-m,p-q}(iq)\,|q|^{n-1-m}\,a_{m,q}, \quad (6)$$

where $F'_m(x) := (\partial_x f)F_m(x)$. Together, formulas (5) and (6) can be implemented in a high–level computing language to deliver a fast and accurate method for simulating the action of the DNO, $G : \xi \to \nu$.

4 The Method of Operator Expansions

The second HOPS approach we investigate considers the DNO alone without explicit reference to the underlying field equations. For this reason the method has been termed the method of Operator Expansions (OE). The first *high–order* implementation for electromagnetics (the Helmholtz equation) is due to Milder [Mil91a, Mil91b] and Milder & Sharp [MS91, MS92]. The first *high–order* implementation for water waves (the Laplace equation) is due to Craig & Sulem [CS93]. Once again, we use, in a fundamental way, the representation, (2),

$$v(x,y) = \sum_{p=-\infty}^{\infty} a_p e^{|p|y} e^{ipx}.$$

This HOPS method uses the fact that, for a boundary perturbation $g(x) = \varepsilon f(x)$, the DNO, $G = G(\varepsilon f)$, depends *analytically* upon ε.

Again, assume that the interface is shaped by $g(x) = \varepsilon f(x)$ where $f \sim \mathscr{O}(1)$ and, initially, $\varepsilon \ll 1$. We now focus on the definition of the DNO, G,

$$G(g)[\xi] = \nu,$$

and seek the action of G on a *basis function*, $\exp(ipx)$. To achieve this we use a bounded, periodic solution of Laplace's equation

$$v_p(x,y) := e^{|p|y} e^{ipx}. \quad (7)$$

Inserting the solution $v_p(x,y)$ into the definition of the DNO gives

$$G(g)[v_p(x,g(x))] = [\partial_y v_p - (\partial_x g)\partial_x v_p]_{y=g(x)}.$$

We assume that everything is *analytic* in ε and expand

$$\left(\sum_{n=0}^{\infty} \varepsilon^n G_n(f)\right) \left[\sum_{m=0}^{\infty} \varepsilon^m F_m |p|^m e^{ipx}\right] = \sum_{n=0}^{\infty} \varepsilon^n F_n |p|^{n+1} e^{ipx} \\ - \varepsilon(\partial_x f) \sum_{n=0}^{\infty} \varepsilon^n F_n(ip) |p|^n e^{ipx}.$$

At $\mathscr{O}\left(\varepsilon^0\right)$ this reads

$$G_0\left[e^{ipx}\right] = |p| e^{ipx},$$

so that we can conclude that

$$G_0[\xi] = G_0\left[\sum_{p=-\infty}^{\infty} \hat{\xi}_p e^{ipx}\right] = \sum_{p=-\infty}^{\infty} \hat{\xi}_p G_0\left[e^{ipx}\right] = \sum_{p=-\infty}^{\infty} |p| \hat{\xi}_p e^{ipx} =: |D| \xi,$$

which defines the order–one Fourier multiplier $|D|$. At order $\mathscr{O}(\varepsilon^n)$, $n > 0$, we find

$$\sum_{m=0}^{n} G_m(f)\left[F_{n-m} |p|^{n-m} e^{ipx}\right] = F_n |p|^{n+1} e^{ipx} - (\partial_x f) F_{n-1}(ip) |p|^{n-1} e^{ipx},$$

which we can write as

$$G_n(f)\left[e^{ipx}\right] = F_n |p|^{n+1} e^{ipx} - (\partial_x f) F_{n-1}(ip) |p|^{n-1} e^{ipx} \\ - \sum_{m=0}^{n-1} G_m(f)\left[F_{n-m} |p|^{n-m} e^{ipx}\right].$$

or, using $\partial_x e^{ipx} = (ip) e^{ipx}$,

$$G_n(f)\left[e^{ipx}\right] = F_n |D|^{n+1} e^{ipx} - (\partial_x f) F_{n-1} \partial_x |D|^{n-1} e^{ipx} \\ - \sum_{m=0}^{n-1} G_m(f)\left[F_{n-m} |D|^{n-m} e^{ipx}\right].$$

Since $(ip)^2 = -|p|^2$ we deduce that $|D|^2 = -\partial_x^2$ and we arrive at

$$G_n(f)\left[e^{ipx}\right] = \left(-F_n \partial_x^2 - (\partial_x f) F_{n-1} \partial_x\right) |D|^{n-1} e^{ipx} \\ - \sum_{m=0}^{n-1} G_m(f)\left[F_{n-m} |D|^{n-m} e^{ipx}\right].$$

Next, since

$$\partial_x \left[F_n \partial_x J\right] = F_n \partial_x^2 J + (\partial_x f) F_{n-1} \partial_x J,$$

we have

$$G_n(f)\left[e^{ipx}\right] = -\partial_x F_n \partial_x |D|^{n-1} e^{ipx} - \sum_{m=0}^{n-1} G_m(f)\left[F_{n-m} |D|^{n-m} e^{ipx}\right].$$

As we have the "action" of G_n on any complex exponential $\exp(ipx)$, we write down the *Slow OE Recursions*

$$G_n(f)[\xi] = -\partial_x F_n \partial_x |D|^{n-1} \xi - \sum_{m=0}^{n-1} G_m(f)\left[F_{n-m} |D|^{n-m} \xi\right], \tag{8}$$

for any function

$$\xi(x) = \sum_{p=-\infty}^{\infty} \hat{\xi}_p e^{ipx}.$$

So, what is wrong with this set of recursions, (8)? To compute G_n one must evaluate G_{n-1}, which requires the application of G_{n-2}, etc. Since the *argument* of G_m *changes* as m changes, these cannot be precomputed and stored. Therefore, a naive implementation will require time proportional to $\mathscr{O}(n!)$. One can improve this by storing G_m as an *operator* (a matrix in finite dimensional space), and thus computing G_n requires time proportional to $\mathscr{O}\left(nN_x^2\right)$. Happily we can do even better by using the *self–adjointness* properties of the DNO.

It can be shown that the DNO, G, and all of its Taylor series terms G_n are *self–adjoint*: $G^* = G$ and $G_n^* = G_n$. This can be used to advantage by recalling that $(AB)^* = B^* A^*$, $\partial_x^* = -\partial_x$, and $F_n^* = F_n$. Now, one takes the adjoint of G_n to realize the *Fast OE Recursions*

$$G_n(f)[\xi] = G_n^*(f)[\xi] = -|D|^{n-1} \partial_x F_n \partial_x \xi - \sum_{m=0}^{n-1} |D|^{n-m} F_{n-m} G_m(f)[\xi]. \tag{9}$$

As above, formula (9) can be implemented on a computer to deliver an alternative, fast and accurate method for simulating the action of the DNO, $G : \xi \to \nu$.

5 Numerical Tests

Now that we have *two* HOPS schemes for approximating DNOs, we can test them and compare their performance. For this we make use of the following exact solution. Recall the solution we used for the OE formula

$$v_p(x,y) := e^{|p|y} e^{ipx}.$$

If we choose a wavenumber, say r, and a profile $f(x)$, for a given $\varepsilon > 0$, it is easy to see that the Dirichlet data

$$\xi_r(x;\varepsilon) := v_r(x,\varepsilon f(x)) = e^{|r|\varepsilon f(x)} e^{irx}$$

generates Neumann data

$$\begin{aligned} v_r(x;\varepsilon) &:= \left[\partial_y v_r - \varepsilon(\partial_x f)\partial_x v_r\right](x,\varepsilon f(x)) \\ &= \left[|r| - \varepsilon(\partial_x f)(ir)\right] e^{|r|\varepsilon f(x)} e^{irx}. \end{aligned}$$

Using this we can, with a Fourier spectral method in mind [GO77, CHQZ88], sample the ξ_r at equally spaced points, appeal to either the FE or OE algorithms described above, and compare our outputs to ν_r evaluated at these same gridpoints.

To be more specific, for either HOPS algorithm we choose a number of equally–spaced collocation points, N_x, and perturbation orders, N. For the FE algorithm we utilize (5) to find approximations $a_{n,p}^{N_x}$ for $-N_x/2 \le p \le N_x/2-1$ and $0 \le n \le N$ and form

$$\nu_{FE}^{N_x,N}(x) := \sum_{n=0}^{N} \sum_{p=-N_x/2}^{N_x/2-1} a_{n,p}^{N_x} e^{ipx} \varepsilon^n. \tag{10}$$

All nonlinearities are approximated on the physical side using pointwise multiplication, while Fourier multipliers are implemented in wavenumber space by invoking an FFT, applying the (diagonal) Fourier multiplier operator, and then appealing to the inverse FFT algorithm. In the same way, the OE method uses (9) to provide approximations $\nu_{n,p}^{Nx}$ which are then used to generate $\nu_{OE}^{N_x,N}$ just as in (10).

We consider a problem with geometric and numerical parameters

$$L = 2\pi, \quad \varepsilon = 0.02, \quad f(x) = \exp(\cos(x)), \quad N_x = 64, \quad N = 16, \tag{11}$$

and note that f is real analytic and that all of its derivatives are $L = 2\pi$–periodic (so that its Fourier series decays exponentially fast). In Figure 1 we display results of our numerical experiments with the FE algorithm as N is refined from 0 to 16. We repeat this in Figure 2 for the OE recursions, and plot them together in Figure 3. Here we note the stable and rapid convergence one can realize with this algorithm as the perturbation order N is increased.

6 Generalizations

Having described two rather simple and efficient algorithms for the simulation of solutions to Laplace's equation on a semi–infinite domain in two dimensions, one can ask, are these algorithms restricted to this simple case? Happily we can answer in the negative and now describe how to generalize the algorithms to three dimensions (§ 6.1) and finite depth (§ 6.2). Other generalizations are possible (e.g., to Helmholtz [NR04a, NR04b, MN11] and Maxwell [BR93c, Nic14] equations, and the equations of elasticity [FN14]) but would take us rather far afield.

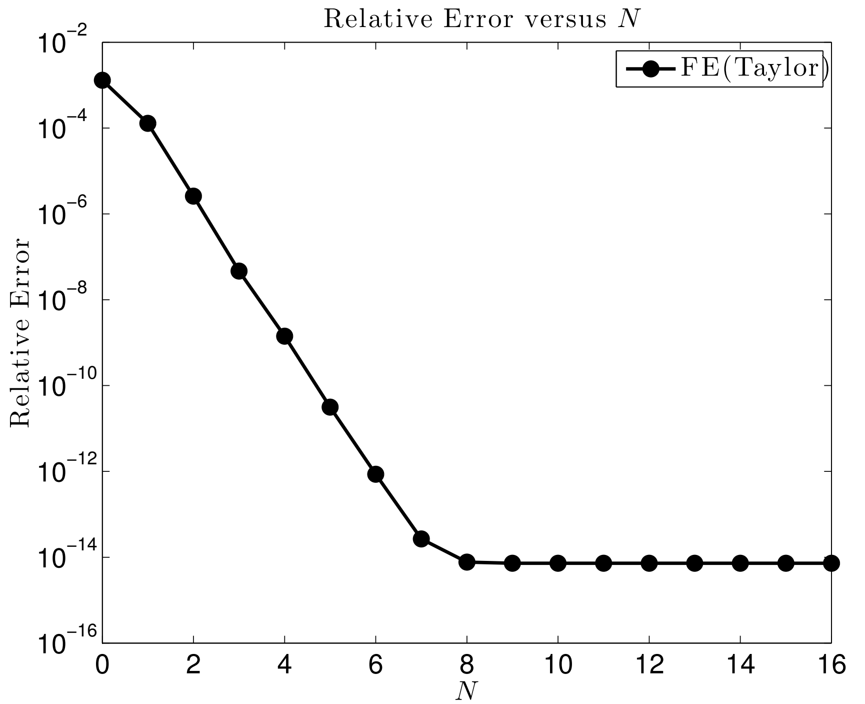

Fig. 1 Relative error in FE algorithm versus perturbation order N for smooth interface configuration, (11), with Taylor summation.

6.1 Three Dimensions

A generalization of crucial importance is to the more realistic situation of a genuinely three–dimensional fluid. In this case the air–fluid interface, $y = g(x) = g(x_1, x_2)$ is two–dimensional rather than one–dimensional. Such a generalization for Boundary Integral/Element methods requires a new formulation as the fundamental solution changes from

$$\Phi_2(r) = C_2 \ln(r),$$

to

$$\Phi_3(r) = C_3 r^{-1}.$$

One of the most appealing features of our HOPS methods is the *trivial* nature of the changes required moving from two to three dimensions. This can be seen by inspecting the solution of Laplace's equation, c.f. (2),

$$v(x,y) = \sum_{p_1=-\infty}^{\infty} \sum_{p_2=-\infty}^{\infty} a_p e^{|p|y} e^{ip\cdot x}, \quad p = (p_1, p_2) \in \mathbf{Z}^2.$$

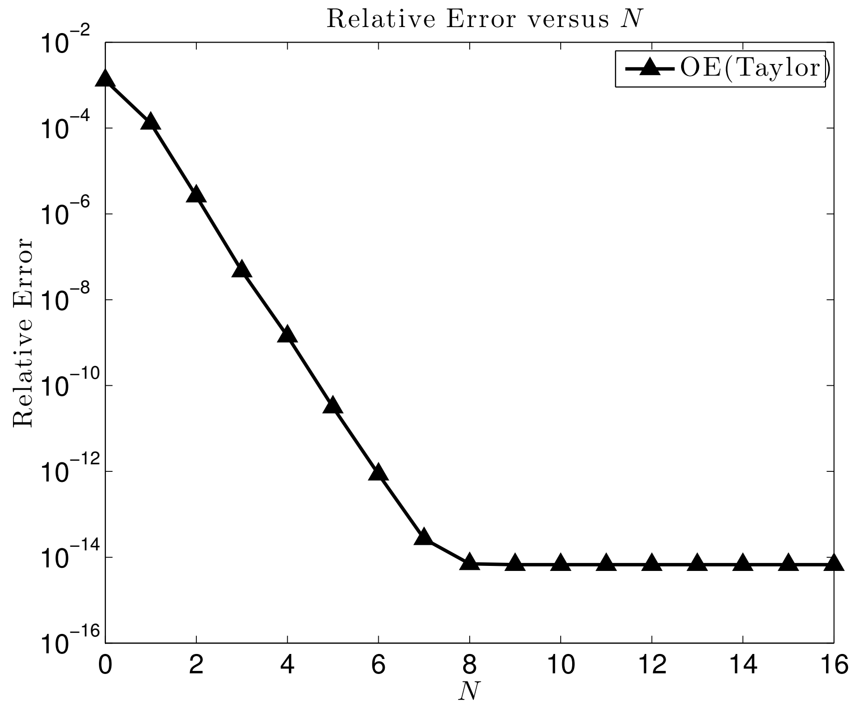

Fig. 2 Relative error in OE algorithm versus perturbation order N for smooth interface configuration, (11), with Taylor summation.

Once again assuming $g(x_1,x_2) = \varepsilon f(x_1,x_2)$, $f \sim \mathscr{O}(1)$, $\varepsilon \ll 1$, we expand

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

We find the same inhomogeneous Laplace problem, (3), at every perturbation order n which has solution, c.f. (4),

$$v_n(x,y) = \sum_{p_1=-\infty}^{\infty} \sum_{p_2=-\infty}^{\infty} a_{n,p} e^{|p|y} e^{ip\cdot x}.$$

Following the development from before we find, c.f. (5),

$$a_{n,p} = \delta_{n,0}\hat{\xi}_p - \sum_{m=0}^{n-1} \sum_{q_1=-\infty}^{\infty} \sum_{q_2=-\infty}^{\infty} \hat{F}_{n-m,p-q} \, |q|^{n-m} \, a_{m,q}.$$

As before, if we seek the Neumann data

$$\nu(x) = \left[\partial_y v - (\partial_x g)\partial_x v\right]_{y=g(x)},$$

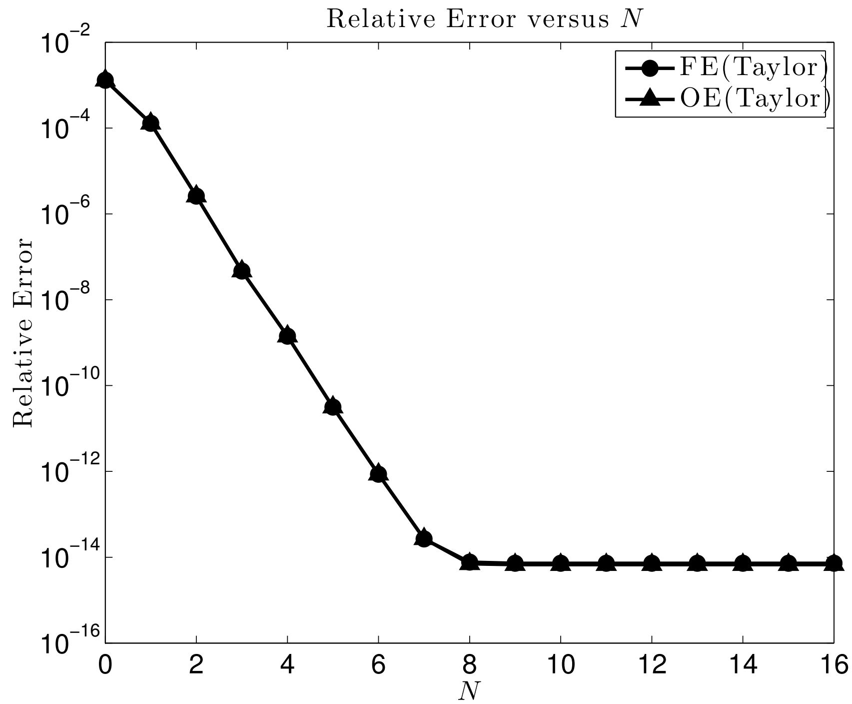

Fig. 3 Relative error in FE and OE algorithms versus perturbation order N for smooth interface configuration, (11), with Taylor summation.

and expand

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

then FE delivers approximations to v_n from the $a_{n,p}$. More precisely, for $F'_m(x) := (\nabla_x f)F_m(x)$, c.f. (6),

$$\hat{v}_{n,p} = \sum_{m=0}^{n} \sum_{q_1=-\infty}^{\infty} \sum_{q_2=-\infty}^{\infty} \hat{F}_{n-m,p-q} \, |q|^{n+1-m} \, a_{m,q} - \sum_{m=0}^{n-1} \sum_{q_1=-\infty}^{\infty} \sum_{q_2=-\infty}^{\infty} \hat{F}'_{n-1-m,p-q} \cdot (iq) \, |q|^{n-1-m} \, a_{m,q},$$

Regarding the OE methodology, we once again assume that the interface is shaped by $g(x_1,x_2) = \varepsilon f(x_1,x_2)$, $f \sim \mathscr{O}(1)$, $\varepsilon \ll 1$. As before, we seek the *action* of G on a basis function, $\exp(ip \cdot x)$. To achieve this we use a bounded, periodic solution of Laplace's equation, c.f. (7),

$$v_p(x,y) := e^{|p|y} e^{ip\cdot x}.$$

We make the expansion

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

and seek forms for the G_n. Using the methods outlined ealier, we can show that

$$G_0[\xi] = |D|\,\xi = \sum_{p_1=-\infty}^{\infty} \sum_{p_2=-\infty}^{\infty} |p|\,\hat{\xi}_p e^{ip\cdot x},$$

and, for $n > 0$,

$$G_n(f)[\xi] = -\mathrm{div}_x \left[F_n \nabla_x |D|^{n-1} \xi\right] - \sum_{m=0}^{n-1} G_m(f) \left[F_{n-m} |D|^{n-m} \xi\right],$$

c.f. (8). Again, these can be accelerated by *adjointness* considerations to

$$G_n(f)[\xi] = -|D|^{n-1} \mathrm{div}_x [F_n \nabla_x \xi] - \sum_{m=0}^{n-1} |D|^{n-m} F_{n-m} G_m(f)[\xi],$$

c.f. (9).

6.2 Finite Depth

As we will now show, the generalization to *finite depth* is immediate. The problem statement, (1), is the same, save we replace $\partial_y v \to 0$ with

$$\partial_y v(x,-h) = 0.$$

Once again, the key is the periodic solution of Laplace's equation satisfying this boundary condition, c.f. (7),

$$v_p(x,y) := \frac{\cosh(|p|(y+h))}{\cosh(|p|h)} e^{ipx}.$$

Since v_p and $\partial_y v_p$ *evaluated at* $y = 0$ will clearly become important, we introduce the symbol

$$T_{n,p} = T_{n,p}(h) := \begin{cases} 1 & n \text{ even} \\ \tanh(h|p|) & n \text{ odd} \end{cases}.$$

We can show that the *FE Recursions* become

$$a_{p,n} = \delta_{n,0}\hat{\xi}_p - \sum_{m=0}^{n-1} \sum_{q=-\infty}^{\infty} \hat{F}_{n-m,p-q} |q|^{n-m} T_{n-m,q}(h) a_{m,q},$$

c.f. (5), and that

$$\hat{v}_{n,p} = \sum_{m=0}^{n} \sum_{q=-\infty}^{\infty} \hat{F}_{n-m,p-q} \, |q|^{n+1-m} \, T_{n+1-m}(h) a_{m,q} \\ - \sum_{m=0}^{n-1} \sum_{q=-\infty}^{\infty} \hat{F}'_{n-1-m,p-q}(iq) \, |q|^{n-1-m} \, T_{n-1-m}(h) a_{m,q},$$

c.f. (6).

For the OE recursions we can show that, at order zero,

$$G_0[\xi] = \sum_{p=-\infty}^{\infty} |p| \tanh(h|p|) \hat{\xi}_p e^{ipx} = |D| \tanh(h|D|) \xi,$$

while at higher orders (after appealing to *self–adjointness*)

$$G_n(f)[\xi] = -|D|^{n-1} T_{n+1,D} \partial_x F_n \partial_x \xi - \sum_{m=0}^{n-1} |D|^{n-m} T_{n-m,D} F_{n-m} G_m(f)[\xi],$$

c.f. (9).

7 Padé Summation

One of the classical problems of numerical analysis is the approximation of an analytic function given a truncation of its Taylor series. Simply evaluating the truncation will be spectrally accurate in the number of terms for points *inside* the disk of convergence of the Taylor series. However, one may be interested in points of analyticity *outside* this disk, and a numerical "analytic continuation" is of great interest. Padé approximation [BGM96] is one of the most popular and successful choices for this procedure, and we refer the interested reader to the insightful calculations of § 8.3 of Bender & Orszag [BO78] for more details.

To summarize this procedure, consider the analytic function

$$c(\varepsilon) = \sum_{n=0}^{\infty} c_n \varepsilon^n$$

which we approximate by its truncated Taylor series

$$c^N(\varepsilon) := \sum_{n=0}^{N} c_n \varepsilon^n.$$

If ε_0 is in the disk of convergence then

$$\left| c(\varepsilon_0) - c^N(\varepsilon_0) \right| < K \rho^N.$$

However, if ε_0 is a point of analyticity *outside* the disk of convergence of the Taylor series, c^N will produce *meaningless* results.

The idea behind Padé summation is to approximate c^N by the rational function

$$[L/M](\varepsilon) := \frac{a^L(\varepsilon)}{b^M(\varepsilon)} = \frac{\sum_{l=0}^{L} a_l \varepsilon^l}{\sum_{m=0}^{M} b_m \varepsilon^m}$$

where $L+M=N$ and

$$[L/M](\varepsilon) = c^N(\varepsilon) + \mathscr{O}\left(\varepsilon^{L+M+1}\right).$$

For convenience we choose the *equiorder* Padé approximant $[N/2,N/2](\varepsilon)$. For the purposes of the following discussion we assume that either N is even or, in the case N odd, that the highest–order term c_N is ignored so that $L=M=N/2$ is an integer.

To derive equations for the $\{a_l\}$ and $\{b_m\}$ we note that

$$\frac{a^M(\varepsilon)}{b^M(\varepsilon)} = c^{2M}(\varepsilon) + \mathscr{O}\left(\varepsilon^{2M+1}\right)$$

is equivalent to

$$b^M(\varepsilon)c^{2M}(\varepsilon) = a^M(\varepsilon) + \mathscr{O}\left(\varepsilon^{2M+1}\right),$$

or

$$\left(\sum_{m=0}^{M} b_m \varepsilon^m\right)\left(\sum_{n=0}^{2M} c_n \varepsilon^n\right) = \left(\sum_{m=0}^{M} a_m \varepsilon^m\right) + \mathscr{O}\left(\varepsilon^{2M+1}\right).$$

Multiplying the polynomials on the left–hand–side and equating at equal orders in ε^m for $0 \le m \le 2M$ reveals two sets of equations

$$\sum_{j=0}^{m} c_{m-j} b_j = a_m \qquad 0 \le m \le M, \tag{12a}$$

$$\sum_{j=0}^{M} c_{m-j} b_j = 0 \qquad M+1 \le m \le 2M. \tag{12b}$$

Given that the c_m are known, if the b_m can be computed then the first equation, (12a), can be used to find the a_m. Without loss of generality we make the classical specification $b_0 = 1$ so that the second equation, (12b), becomes

$$\sum_{j=1}^{M} c_{m-j} b_j = -c_m, \quad M+1 \le m \le 2M,$$

or $H\tilde{b} = -r$ where

$$H = \begin{pmatrix} c_M & \dots & c_1 \\ c_{M+1} & \dots & c_2 \\ \vdots & \ddots & \vdots \\ c_{2M-1} & \dots & c_M \end{pmatrix}, \quad \tilde{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_M \end{pmatrix}, \quad r = \begin{pmatrix} c_{M+1} \\ c_{M+2} \\ \vdots \\ c_{2M} \end{pmatrix}.$$

To see the extremely beneficial effects this procedure can have upon HOPS simulations, we revisit the calculations of § 5 save that we consider a deformation of size $\varepsilon = 0.2$ (ten times as large). More specifically, we once again consider the problem (11) (with $\varepsilon = 0.2$) and compare Taylor summation with Padé approxmation. In Figures 4 and 5 we show the discouraging results delivered by FE and OE in this challenging configuration with Taylor summation. However, as we display in Figure 6 one is able to recover nearly full double precision from the FE and OE approximations of the Taylor coefficients provided one appeals to the analytic continuation of Padé approximation.

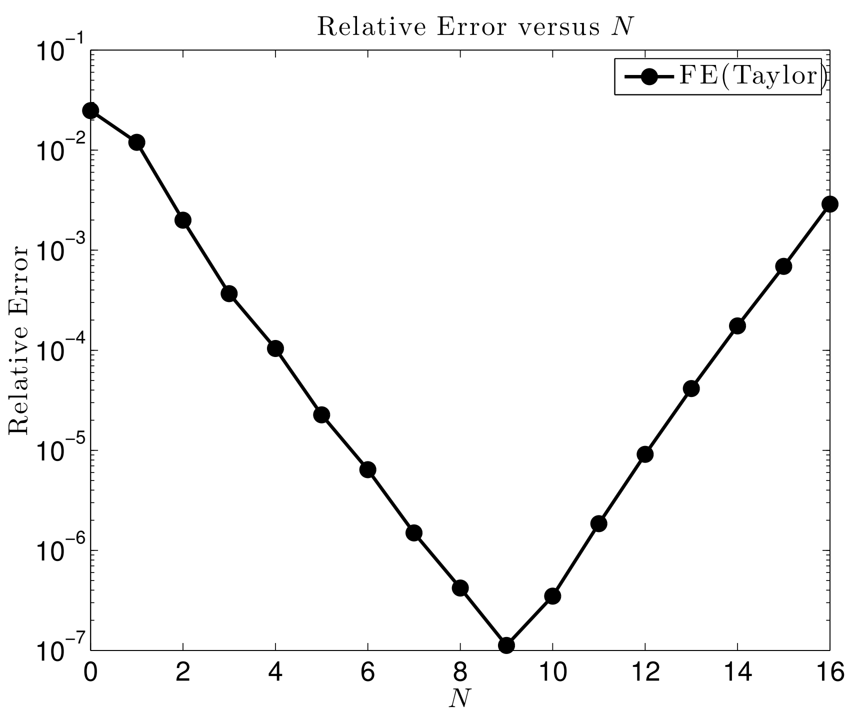

Fig. 4 Relative error in FE algorithm versus perturbation order N for smooth, large interface configuration, (11) ($\varepsilon = 0.2$) with Taylor summation.

Dedication. The author would like to dedicate this contribution to his beautiful wife, Kristy. Without her love and support none of this work would have been possible. This was evident most recently during our family's one–month stay in Cam-

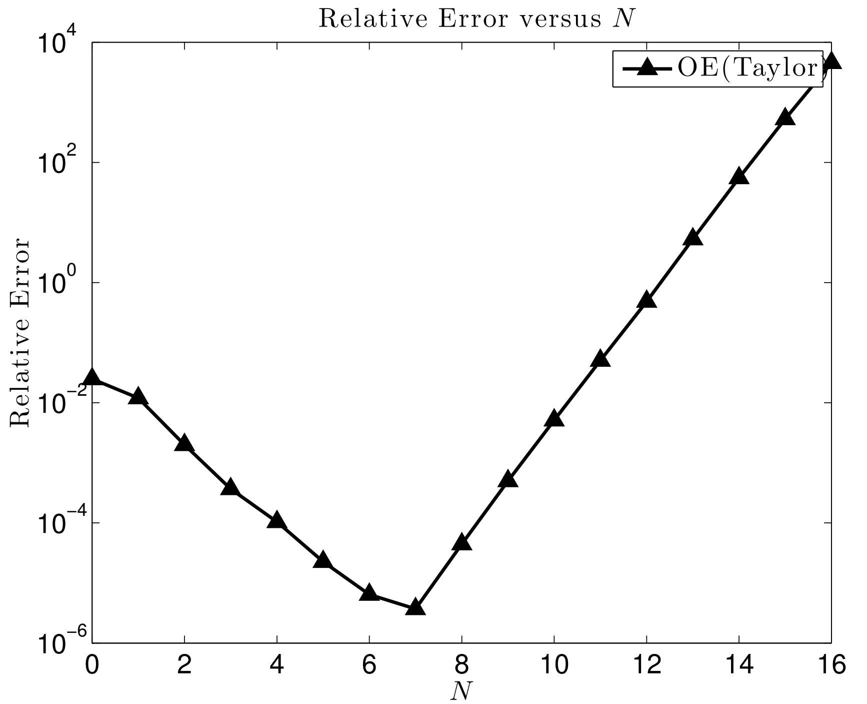

Fig. 5 Relative error in OE algorithm versus perturbation order N for smooth, large interface configuration, (11) ($\varepsilon = 0.2$) with Taylor summation.

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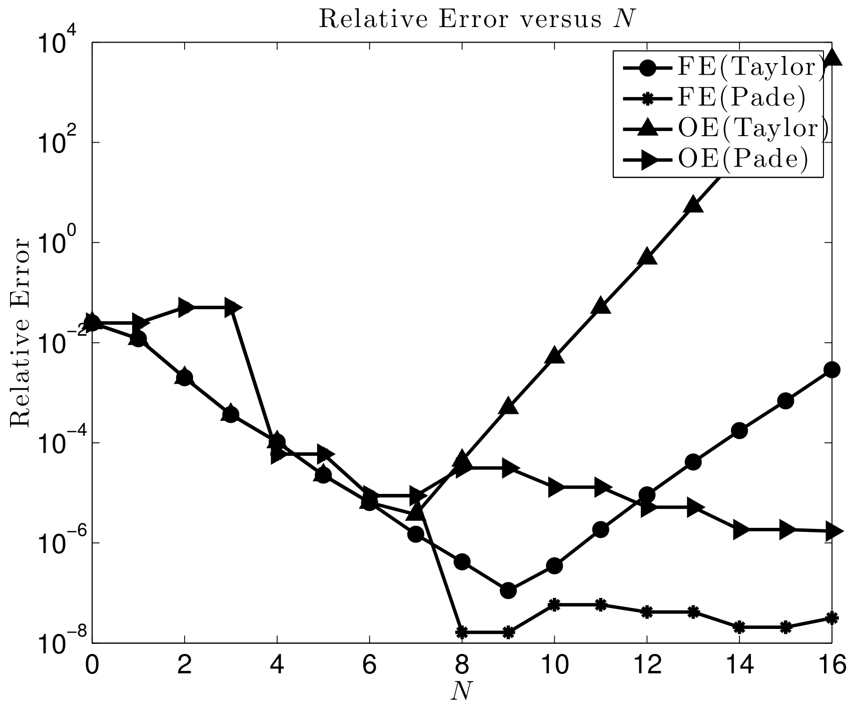

Fig. 6 Relative error in FE and OE algorithms versus perturbation order N for smooth, large interface configuration, (11) ($\varepsilon = 0.2$) with Taylor and Padé summation.

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