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THREE-POINT FINITE-DIFFERENCE SCHEMES, PADÉ AND THE SPECTRAL GALERKIN METHOD. I. ONE-SIDED IMPEDANCE APPROXIMATION

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ABSTRACT. A method for calculating special grid placement for three-point schemes which yields exponential superconvergence of the Neumann to Dirichlet map has been suggested earlier. Here we show that such a grid placement can yield impedance which is equivalent to that of a spectral Galerkin method, or more generally to that of a spectral Galerkin-Petrov method. In fact we show that for every stable Galerkin-Petrov method there is a three-point scheme which yields the same solution at the boundary. We discuss the application of this result to partial differential equations and give numerical examples. We also show equivalence at one corner of a two-dimensional optimal grid with a spectral Galerkin method.

1. INTRODUCTION

The connection between the spectral Galerkin method and finite-difference schemes is well known—it is the essence of the pseudospectral method (for example, see [11]). In the pseudospectral method, one constructs a finite-difference scheme which is equivalent to a Galerkin method for some subspace, for example, a set of algebraic or trigonometric polynomials. Usually such schemes are equivalent to the corresponding Galerkin method in *all finite-difference nodes*, and exponential convergence can be achieved (for regular enough problems) provided the finite-difference stencil (or the matrix of the resulting linear system) is full. Recently in [7, 8, 9] the authors described a method for choosing the placement of the grid points so that by using a *three-point* scheme one can achieve exponential superconvergence at an *endpoint* of the interval.[1] It is known that spectral Galerkin methods can yield sparse matrices [4]; however, the sparsity structures depend on the choice of the subspace. In our approach, the matrix is tridiagonal regardless of the subspace. In other words, we sacrifice spectral convergence everywhere to

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[1]Stricly speaking, depending on the problem, the convergence can be super-geometric, geometric or sub-geometric (geometric of the square root) using terminology of [5], but for simplicity we will combine these into a single term, "exponential" or "spectral" as in the finite-element literature (e.g., [19]).

obtain spectral convergence only at prespecified points with a three-term approximation of second derivatives. In many applications, such as oil exploration, one cares only about convergence at the receiver locations.

One can view this idea as an extension of Gaussian quadrature to second-order finite-difference schemes. A Gaussian k-point quadrature rule for numerical integration is chosen to be exact for $2k$ polynomials, and we choose our k-node grid so that some $2k$ functionals of the solution are exact. The implementation of our finite-difference spectral rules is somehow similar to the implementation of the conventional quadrature rules for numerical integration. It is based on *precomputed* tables of the grids obtained for problems with constant coefficients. In some cases the tabulation is not even needed because the optimal grid can be computed via a simple analytic formula [14]. Then, as was suggested in [2, 9] for wave and elliptic problems with piecewise constant coefficients and rectangular interfaces, the tables are used for the grid generation within every homogeneous subdomain. Another approach is to use a grid which is optimal for constant coefficients for problems with variable coefficients. Such an approach would not produce spectral convergence in a strict sense, but it yields spectral convergence for singular components of the solution [14] which are the most difficult for conventional finite-differences. Thus, at *no cost* this grid optimization approach can be implemented for quite general linear partial differential equations (PDEs). However, at this point it is not clear if it is applicable to nonlinear problems.

Though the grid optimization algorithm and its implementation for some practically interesting problems were covered in the above-mentioned papers [7, 8, 2, 9], the authors used results on rational approximations of Stieltjes functions. Since this approach is not standard in the numerical PDE community, we analyse here the optimal grid technique from the point of view of common *variational* methods.

- We show that for every stable Galerkin (or more generally Galerkin-Petrov) approximation there is a stable three-point finite-difference scheme which generates the same solution at the boundary.
- In particular, we show that the three-point finite-difference scheme based on the simple Padé approximant is equivalent to a polynomial Galerkin method, and also find an equivalent Galerkin-Petrov formulation for the Gaussian difference rules based on the (more efficient) multipoint Padé approximant.

What makes this approach different from the standard high-order approaches is that we do not match the approximation for every grid node, but only for the Neumann to Dirichlet map (also known as the Poincaré-Steklov operator or impedance). This operator is an important tool in the theory and numerical analysis of elliptic PDEs, because it completely describes the coupling of the domain with its neighbours. Using the impedance operator, a large computational domain can be partitioned in simpler subdomains as in the spectral element or multidomain spectral methods [16]. Due to the equivalency of the finite-difference and spectral Galerkin impedance maps, the convergence results for the multidomain spectral method will automatically hold for the finite-difference method at the subsets where these two methods are equivalent. For one-dimensional problems, such subsets are just the boundaries of the subintervals.

By taking the tensor product of optimal grids, one can extend this approach to two or more spatial dimensions, provided the computational domain can be partitioned (by Cartesian interfaces) into rectangular subdomains such that within

every subdomain the variables can be separated. In this case, the subsets where we will have equivalence to a spectral Galerkin method will be the corners of the subdomains. We will discuss this in a second part to this paper [10]. It will provide a rigorous foundation to the implementation of the multidomain optimal grid approach given in [9, 2].

This paper is organized as follows. First we present the model problem in one dimension in Section 2. Then in Section 3 we discuss the optimal grid approach from the point of view of Padé approximation. Section 4 contains a proof that two of the three approaches discussed in Section 3 are equivalent (in terms of an impedance) to conventional Galerkin methods using trigonometric and polynomial subspaces. We also show that every Galerkin approximation has a three-point finite-difference counterpart with the same impedance. In Section 5 we show that the more efficient multipoint Padé approximation has an impedance which is equivalent to a stable Galerkin-Petrov impedance. It is multipoint Padé which is currently being used in applications. In Section 6 we illustrate the application of optimal grids to solving partial differential equations on simple model problems. First we show how one can use one-dimensional optimal grids to greatly improve efficiency for Laplace's equation on a strip and a one-dimensional wave equation. Some of these and other examples have been demonstrated numerically in [2, 14]. Next we prove that by taking the tensor product of a one-dimensional optimal grid with itself, one can obtain a two-dimensional five-point scheme with convergence equivalent to a two dimensional spectral Galerkin method at one corner. Finally, the appendix shows how one could transform the finite-difference solution to the equivalent Galerkin-Petrov solution globally.

In the forthcoming second part to this paper we will use results of the first part along with new results about two-sided impedance approximation to show Galerkin equivalence for some nontrivial two-dimensional problems.

2. Model problem

We consider the one-dimensional problem

$$u''(x) - \lambda u = 0 \tag{1}$$

on the interval $[0, l]$, with boundary conditions

$$-u'(0) = 1$$

and

$$u(l) = 0.$$

(We also include the limit case $l = \infty$.) Let us approximate the solution u to (1) by a staggered three-point finite-difference scheme. In a staggered scheme, the numerical solution is defined at "potential" nodes

$$x_i, \quad i = 1, \ldots, k+1$$

with

$$x_1 = 0$$

and

$$x_{i+1} > x_i,$$

and the finite-difference derivatives are defined at "derivative" nodes

$$\hat{x}_i, \quad i = 0, \ldots, k,$$

with

$$\hat{x}_0 = 0.$$

We denote the step sizes by

$$h_i = x_{i+1} - x_i$$

and

$$\hat{h}_i = \hat{x}_i - \hat{x}_{i-1},$$

and solve the finite-difference problem

$$\frac{1}{\hat{h}_i}\left(\frac{w_{i+1} - w_i}{h_i} - \frac{w_i - w_{i-1}}{h_{i-1}}\right) - \lambda w_i = 0, \qquad i = 2, \ldots, k, \tag{2}$$

with boundary conditions

$$\frac{1}{\hat{h}_1}\left(\frac{w_2 - w_1}{h_1}\right) - \lambda w_1 = -\frac{1}{\hat{h}_1}$$

and

$$w_{k+1} = 0.$$

Note that the first boundary condition is consistent with the differential equation since it is the same as creating a dummy node w_0, allowing $i = 1$ in (2) and setting

$$-\frac{w_1 - w_0}{h_0} = 1.$$

We express the linear system (2) for w in shorthand by

$$(L_h - \lambda)w = -\frac{1}{\hat{h}_1}e_1, \tag{3}$$

where e_1 is the unit vector with support in the first component. The continuous, or true, impedance function $f(\lambda)$ is defined by

$$f(\lambda) \equiv u(0),$$

and the discrete, or approximate, impedance function $f_k(\lambda)$ is defined by

$$f_k(\lambda) \equiv w_1.$$

Our objective is to choose the placement of the grid points so that the discrete impedance function $f_k(\lambda)$ is an accurate approximation to $f(\lambda)$ on some interval of possible frequencies λ. We will a priori require that the step sizes h_i and $\hat{h}_i$ be positive to ensure the stability of (2).

3. Padé approach

Suppose we approximate the solution to (1) by the finite difference solution to (3). Then, as the next lemma shows us, we can represent the discrete impedance in terms of the eigenpairs of the matrix L_h. Note that L_h is not symmetric in the standard sense, but is symmetric with respect to the inner product with weights $\hat{h}_i$,

$$\langle x, y \rangle_{\hat{h}} = \sum_{i=1}^{k} \hat{h}_i x_i y_i,$$

that is

$$\langle L_h x, y \rangle_{\hat{h}} = \langle x, L_h y \rangle_{\hat{h}}$$

for any $x, y \in R^k$. In addition, for any nontrivial x,

$$\langle L_h x, x \rangle_{\hat{h}} < 0.$$

Hence, L_h has a real eigendecomposition with negative eigenvalues.

Lemma 1. *Let z_i, θ_i be the eigenvectors and eigenvalues, respectively, of the matrix L_h, normalized with respect to the inner product $\langle , \rangle_{\hat{h}}$. Then the discrete impedance function can be written as*

$$f_k(\lambda) = \sum_{i=1}^{k} \frac{y_i}{\lambda - \theta_i}, \tag{4}$$

where

$$y_i = (z_i)_1^2.$$

Proof. Since the eigenvectors z_i form an $\hat{h}$ orthonormal basis for $\Re^k$, we can decompose the finite-difference solution w into

$$w = \sum_{i=1}^{k} \langle w, z_i \rangle_{\hat{h}} z_i$$

so that its first component (or the discrete impedance) is

$$w_1 = \sum_{i=1}^{k} \langle w, z_i \rangle_{\hat{h}} (z_i)_1. \tag{5}$$

Now, using the fact that (z_i, θ_i) is an eigenpair of L_h,

$$\begin{aligned} \langle w, z_i \rangle_{\hat{h}} &= \langle w, \frac{1}{\theta_i} L_h z_i \rangle_{\hat{h}} \\ &= \frac{1}{\theta_i} \langle L_h w, z_i \rangle_{\hat{h}}. \end{aligned}$$

Due to (3), we further calculate that

$$\begin{aligned} \langle w, z_i \rangle_{\hat{h}} &= \frac{1}{\theta_i} \langle \lambda w, z_i \rangle_{\hat{h}} - \frac{1}{\theta_i} \langle \frac{1}{\hat{h}_1} e_1, z_i \rangle_{\hat{h}} \\ &= \frac{1}{\theta_i} \langle \lambda w, z_i \rangle_{\hat{h}} - \frac{1}{\theta_i} (z_i)_1, \end{aligned}$$

which implies that

$$\langle w, z_i \rangle_{\hat{h}} = \frac{(z_i)_1}{\lambda - \theta_i}.$$

The lemma follows from inserting this into (5). □

Lemma 1 says that for any stable finite-difference scheme the impedance function can be represented as (4) with negative poles and positive residues, i.e., it states a necessary condition for a rational function of the form (4) to be a finite-difference impedance function. The following lemma shows that this condition is also sufficient.

Lemma 2 (Stieltjes, Kac-Krein). *Any rational function of the form* (4) *with negative noncoinciding poles and positive residues is the impedance function of a k-node finite-difference scheme with positive steps.*

The well-known mechanical equivalent of the finite-difference scheme is the string of point masses $\hat{h}_i$ connected by weightless springs with stiffnesses h_i, and for such a string the proof of the lemma can be found in [15] (see also [3, Theorem 5.1.2, Corollary 2]). The proof is based on the Stieltjes continued fraction representation of f_k, that is

$$f_k(\lambda) = \cfrac{1}{\hat{h}_1\lambda + \cfrac{1}{h_1 + \cfrac{1}{\hat{h}_2\lambda + \ldots \cfrac{1}{h_{k-1} + \cfrac{1}{\hat{h}_k\lambda + \cfrac{1}{h_k}}}}}}. \tag{6}$$

Given an impedance function of the form (4), from parameters y_i and θ_i we can obtain the step sizes h_i and $\hat{h}_i$ by equating (4) to (6) and using the Euclid polynomial division algorithm. Stable excecution can be done with the help of the Lanczos method with reorthogonalization, which results in $O(k^3)$ arithmetical operations (see [17, 9] for the details of this process). As was mentioned in the introduction, the grids are computed only once a priori and one just uses their tables when actually computing PDE solutions. Thus the grid generation does not add to the cost of the implementation. The idea of [7] was to choose these poles and residues (y_i and θ_i) so that (4) is an accurate approximation to the true impedance function $f(\lambda)$, and then to find the step sizes h_i and $\hat{h}_i$ that correspond to this approximation $f_k(\lambda)$.

Since there is a one-to-one correspondence between finite-difference approximations with positive steps (2) and rational sums (4) with noncoinciding nonpositive poles θ_i and positive residues y_i [15], we need to impose corresponding constraints on the poles and the residues when we find an approximation to $f(\lambda)$. We will call the approximants satisfying these constraints "stable" since they provide stability of the underlying finite-difference scheme. All the approximants considered below will automatically satisfy these constraints.

Solving (1) analytically, we obtain the formula for the true impedance function

$$f(\lambda) = \frac{\tanh(l\sqrt{\lambda})}{\sqrt{\lambda}}.$$

This function, as well as the stable finite-difference impedance f_k, are Stieltjes functions[2] of λ. That is, they can be written as

$$f(\lambda) = \int_{-\infty}^{0} (\lambda - \gamma)^{-1} \, d\sigma(\gamma),$$

where $\sigma(\lambda)$ is some positive (spectral) measure on $(-\infty, 0]$ such that the integral converges. For the finite-difference impedance f_k we have that

$$\frac{d}{d\lambda}\sigma(\lambda) = \sum_{i=1}^{k} y_i \delta(\lambda - \theta_i).$$

For the true impedance on bounded intervals ($l < \infty$), the spectral measure is also discrete,

$$\frac{d}{d\lambda}\sigma(\lambda) = \frac{2}{l} \sum_{i=1}^{\infty} \delta(\lambda - \omega_i),$$

where

$$\omega_i = -\left[\frac{\pi(i - 1/2)}{l}\right]^2$$

are the eigenvalues of (1). If the interval is unbounded ($l = \infty$), the spectrum of the true impedance is continuous. The measure is given by

$$\sigma(\lambda) = -2\pi\sqrt{-\lambda}.$$

We will therefore attempt to apply the well-developed theory of Padé approximants to Stieltjes functions (see, for example, [3, 13]). That is, since $f(\lambda)$ is a Stieltjes function, we will choose residues and poles y_i, θ_i such that the discrete impedance $f_k(\lambda)$ is a Padé approximant to $f(\lambda)$.

Before discussing the Padé approximants in more detail, we should note that for the case of the bounded interval we could approximate the true impedance by simply truncating its multipole expansion

$$f(\lambda) = \frac{2}{l} \sum_{i=1}^{\infty} \frac{1}{\lambda - \omega_i}.$$

That is, we could take

$$f_k(\lambda) = \frac{2}{l} \sum_{i=1}^{k} \frac{1}{\lambda - \omega_i}. \tag{7}$$

This approach yields only algebraic convergence, but it can be useful in combination with a Padé approximant for wave problems. We will use (7) to partially eliminate the spectrum.

We will now discuss two main types of Padé approximants:

[2]More precisely, they are Markov functions of λ; however, since any Markov function can be transformed to a more familiar Stieltjes form, we will refer to f as a Stieltjes function.

1. Simple Padé approximant

$$\frac{d^i}{d\lambda^i}\left[f_k(\lambda) - f(\lambda)\right]\Big|_{\lambda=b} = 0, \qquad i = 0, \dots, 2k-1, \tag{8}$$

for some b outside the spectrum of (1).

2. Multipoint Padé approximant

$$\left[f_k(\lambda) - f(\lambda)\right]|_{\lambda=b_i} = 0, \qquad i = 1, \dots, 2k, \tag{9}$$

where $b_1 < b_2 < \cdots < b_{2k}$ are outside of the spectrum of (1).

We may use either of the above Padé approximants (8) or (9) to define $f_k(\lambda)$, and in either case $f_k(\lambda)$ will converge to $f(\lambda)$ at least exponentially in k for λ outside of the spectrum of (1). In addition, both approximants will produce (4) with noncoinciding negative θ_i and positive y_i [3, 13]. One can view this idea as an extension of Gaussian quadrature to second-order finite-difference schemes. A Gaussian k-point quadrature rule for numerical integration is chosen to be exact for $2k$ polynomials, and we chose our k-node grid so that the impedance satisfies $2k$ matching equations (8) or (9). Thus the Gaussian finite-difference rules yield exponential superconvergence at the boundary for the solution of (2).

Remark. The convergence rates of f_k to f for the Padé approximants depend on the points b or b_i and the logarithmical capacity of the spectrum of (1) [3]. For $l < \infty$, the spectral measure is discrete and hence has logarithmical capacity zero, so the convergence is actually *superexponential.* If $l = \infty$, the spectrum is continuous with a bounded positive logarithmical capacity, and the convergence will be exponential. The approximation error of (8) grows rapidly away from b, so the multipoint Padé approximants with a proper choice of b_i have better approximation properties for λ on an interval of the real axis, i.e., $\lambda \in [\lambda_1, \lambda_2]$. For example, in the Padé-Chebyshev approximant, f_k is defined by the conditions

$$\int_{\lambda_1}^{\lambda_2} \lambda^i \left(f_k(\lambda) - f(\lambda)\right) \rho(\lambda) d\lambda = 0 \qquad \text{for} \quad i = 0, \dots, 2k-1, \tag{10}$$

where

$$\rho(\lambda) = \left(1 - \left[\frac{2\lambda - (\lambda_2 + \lambda_1)}{\lambda_2 - \lambda_1}\right]^2\right)^{-1/2}$$

is the Chebyshev spectral weight adjusted to $[\lambda_1, \lambda_2]$. Condition (10) is equivalent to (9) where the b_i are close to the Chebyshev spectral nodes of degree $2k-1$ (see [3]). This is the Padé approximation which was implemented in [2]. Generally, provided the parameters of the both approximants are chosen properly, the approximation error of a simple Padé approximant on a spectral interval $[\lambda_1, \lambda_2]$ with a large condition number $\kappa = \lambda_2/\lambda_1$ is bounded by $Ce^{-4k/\sqrt{\kappa}}$, while the error for the Padé-Chebyshev approximant is bounded by $Ce^{-4k/\sqrt[6]{\kappa}}$ [3].

4. Galerkin formulation

Now we show that the Padé approximant approach (8) to construct f_k is very much related to a Galerkin method. In fact, the Padé approximant (8) is exactly the same as the discrete impedance function obtained from a spectral Galerkin method for (1) with a polynomial subspace.

First we consider the bounded case and for simplicity assume that $l = 1$. Let us define for any $v \in H^1[0,1]$ and positive λ the variational functional

$$\Omega_\lambda(v) = \|v\|^2_{E[0,1]} - 2v(0),$$

where

$$\|v\|^2_{E[0,1]} = \|v'\|^2_{L^2[0,1]} + \lambda\|v\|^2_{L^2[0,1]}$$

is the energy norm. If u is a solution of (1) with $\lambda > 0$, then by integration by parts we can see that

$$f(\lambda) = -\Omega_\lambda(u). \tag{11}$$

Suppose L is some subspace of $H^1[0,1]$. Define the discrete Galerkin impedance function by

$$f_L(\lambda) = -\min_{v\in L,\ v(1)=0} \Omega_\lambda(v). \tag{12}$$

Let $\langle w, v\rangle_E$ be the energy inner product

$$\langle w, v\rangle_E = \int_0^1 w'v' + \lambda \int_0^1 wv.$$

Then if $v = u_L$ is the minimizer in (12), it also satisfies the variational equation

$$\langle v, u_L\rangle_E = v(0) \tag{13}$$

for any $v \in L$. So just as in the continuous case, the impedance function satisfies the energy equality

$$f_L(\lambda) \equiv u_L(0). \tag{14}$$

From the variational equalities we obtain the identity

$$\Omega_\lambda(u_L) - \Omega_\lambda(u) = \|u - u_L\|^2_{E[0,1]}. \tag{15}$$

The identities (11), (14) and (15) combine to give us

Lemma 3. *Let u be the solution to* (1) *and u_L be the Galerkin solution to* (13). *The corresponding impedance functions $f(\lambda)$ and $f_L(\lambda)$ then satisfy*

$$f(\lambda) - f_L(\lambda) = \|u - u_L\|^2_{E[0,1]}.$$

We also need the next lemma which states that the discrete Galerkin impedance $f_L(\lambda)$ could actually be used to generate finite-difference grid steps.

Lemma 4. *The discrete Galerkin impedance $f_L(\lambda)$ produced by variational formulation* (12) *can be written in the form* (4) *with positive y_i and negative noncoinciding θ_i with $k \le \dim(L)$.*

The proof is similar to the proof of Lemma 1. In Lemma 4 the poles θ_i and the residues y_i are, respectively, equal to the Galerkin eigenvalues and the squared values of the Galerkin eigenfunctions at $x = 0$. From Lemmas 2 and 4 we have

Corollary 1. *For any k-dimensional Galerkin approximation there exists a stable three-point finite-difference scheme with no more than k nodes which has the same impedance function.*

Given a Galerkin approximation, one can obtain the equivalent finite difference scheme in two main steps:

(1) Use the Galerkin eigendecomposition to write f_L in the form (4).
(2) Use the algorithm given in [8] to obtain its equivalent representation of the form (6).

Remark. The converse of Corollary 1 is not true. From the variational definition of f_L, it follows that $f_L(\lambda) \leq f(\lambda)$ for all nonnegative λ. multipoint Padé error changes sign for positive λ [13, 3], so it cannot be equal to an impedance function for a Galerkin approximation.

Since the finite-difference system will have the same spectrum as the Galerkin system, the condition number and the stability limitations will be exactly the same for the two methods. Let us first consider the case of the truncated sum (7), which is equivalent to the Fourier method in terms of impedance.

Proposition 1. *Let $f_L(\lambda)$ be the Galerkin impedance corresponding to*

$$L = \text{span}\{\cos(0.5\pi x), \cos(1.5\pi x), \dots, \cos[(k-1/2)\pi x]\},$$

and let f_k be the approximation obtained from (7). Then

$$f_k(\lambda) \equiv f_L(\lambda).$$

Proof. In this case L is exactly the span of the first k eigenfunctions of (1). These functions are also the Galerkin eigenfunctions corresponding to eigenvalues

$$\omega_i = -\pi^2(i-1/2)^2.$$

If we normalize this basis by dividing by $\sqrt{0.5}$, we use the proof of Lemma 1 to obtain that

$$f_L(\lambda) = [\cos(0)/\sqrt{0.5}]^2 \sum_{i=1}^{k} \frac{1}{\lambda - \omega_i}.$$

Hence,

$$f_L(\lambda) = 2 \sum_{i=1}^{k} \frac{1}{\lambda - \omega_i}$$

which is just (7). □

It is well known that the Galerkin solution of Proposition 1 does not converge exponentially to the solution of the nonperiodic two-point problem (1). If instead we were to use polynomial subspaces, we would obtain exponential convergence everywhere on the domain [0,1], and hence for $f_L(\lambda)$. The following proposition shows that (8) is equivalent to a polynomial Galerkin method in terms of impedance.

Proposition 2. *Let*

$$L = \text{span}\left[x-1, (x-1)^3, \dots, (x-1)^{2k+1}\right],$$

let $f_L(\lambda)$ be the Galerkin impedance corresponding to L, and let f_k be the approximation obtained from (8) with $b = 0$. Then

$$f_k(\lambda) \equiv f_L(\lambda).$$

Proof. Solving (1) explicity, we obtain that

$$u(x) = \frac{\sinh\sqrt{\lambda}(x-1)}{\sqrt{\lambda}\cosh\sqrt{\lambda}}.$$

Direct calculation shows that

$$\frac{d^i}{d\lambda^i}u\bigg|_{\lambda=0} \in L \quad \text{for} \quad i = 0, \dots, k-1,$$

which means that the Maclaurin series expansion of u with respect to λ,

$$u_k = \sum_{i=0}^{k-1} \frac{d^i}{d\lambda^i}u\bigg|_{\lambda=0} \frac{\lambda^i}{i!},$$

also belongs to L. So if $v = u_L$ solves (12), then

$$\|u - u_L\|_{E[0,1]} \le \|u - u_k\|_{E[0,1]}.$$

For small λ obviously

$$\|u - u_k\| = O(\lambda^k).$$

Therefore,

$$\|u - u_L\| = O(\lambda^k).$$

Hence, by Lemma 3, we obtain that

$$f(\lambda) - f_L(\lambda) = O(\lambda^{2k}).$$

Also, by Lemma 4, $f_L(\lambda)$ is of the form (4). But by the uniqueness of the Padé approximant, there is only one function of the form (4) which is an $O(\lambda^{2k})$ approximation to $f(\lambda)$ [3, Theorem 1.4.3]. Therefore,

$$f_k(\lambda) \equiv f_L(\lambda).$$

□

For the case $l = \infty$, the Padé approximant (8) with $b = 0$ does not exist since $\lambda = 0$ is in the spectrum of (1). However, it will surely exist for positive b, in which case the Padé approximation will be equivalent to the impedance of the Galerkin solution corresponding to a subspace L consisting of the scaled Laguerre functions $e^{-\sqrt{b}x}p(x)$, where $p(x)$ is a polynomial.

5. Galerkin-Petrov formulation

As follows from (15), the Galerkin impedance function f_L cannot be smaller than the exact impedance f. However, the error function $f_k - f$ of the optimal (on an interval) rational approximant should change sign $2k-1$ times on this interval. Obviously, near optimal approximants, for example, the Padé-Chebyshev approximant [12, 8], also retain this property. Generally such approximants can be described by the multipoint Padé approximant (9), which unlike the simple Padé approximant, cannot be expressed as a Galerkin impedance function. We can, though, express (8) in terms of a variational equality with different trial and test spaces. Suppose we have the test and trial subspaces V and U, respectively. Define the Galerkin-Petrov solution $u_{U,V}$ to be in U and satisfy the equation

$$\langle v, u_{U,V}\rangle_E = v(0) \tag{16}$$

for any $v \in V$, assuming such a solution exists. Then the Galerkin-Petrov impedance function can be defined as

$$f_{U,V} = u_{U,V}(0).$$

One may verify that

$$f_{U,V} = f_{V,U}$$

and

$$f_L = f_{L,L}.$$

Proposition 3. *Let $f_k(\lambda)$ be given by (9), and define a test space*

$$U = \operatorname{span}[q_1, \ldots, q_k]$$

and trial space

$$V = \operatorname{span}[q_{k+1}, \ldots, q_{2k}],$$

with

$$q_i(x) = u(x)|_{\lambda = b_i},$$

where the b_i come from (9). Then the Galerkin-Petrov impedance function $f_{U,V}(\lambda)$ exists, is unique, and

$$f_k(\lambda) \equiv f_{U,V}(\lambda).$$

Proof. When $\lambda = b_i$ for $i = 1, \ldots, k$, U contains the exact solutions. Hence, for these spectral points,

$$u_{U,V} = u$$

and

$$f_{U,V} = f.$$

Similarly, V consists of the exact solutions for the remaining spectral points, so when $\lambda = b_i$ for $i = k+1, \ldots, 2k$,

$$u_{V,U} = u$$

and

$$f_{V,U} = f.$$

But, since

$$f_{V,U} = f_{U,V},$$

we have that

$$f_{U,V}(b_i) = f(b_i) \quad \text{for} \quad i = 1, \ldots, 2k,$$

that is, it satisfies (9). Also, by construction, $f_{U,V}$ can be written in the form (4). So the proposition follows from the existence and uniqueness of the multipoint Padé approximant. □

Lemma 4 with positive residues and negative poles does not generally hold for the Galerkin-Petrov method, but due to the stability of the multipoint Padé approximant [13], the Galerkin-Petrov method of Proposition 3 will be stable.

6. Applications to PDEs

Note that if one has a solution to a partial differential equation of the form

$$\frac{\partial^2 u}{\partial x^2} - Lu = 0,$$

where L is some constant coefficient differential or difference operator in another spatial or temporal variable (or both of them), after taking its (continuous or discrete) Fourier transform in these variables we obtain an equation of the form (1). It is for this reason that the results of the previous sections are directly applicable to the approximation of such PDEs.

6.1. **The Laplace equation.** Let us first consider Laplace's equation on the semi-infinite strip

$$\Omega = [0, \infty] \times [0, 1]$$

given by

$$-\frac{\partial^2 w(x,y)}{\partial y^2} - \frac{\partial^2 w(x,y)}{\partial x^2} = 0 \tag{17}$$

with boundary conditions

$$\left.\frac{\partial w}{\partial x}\right|_{x=0} = -\varphi(y), \qquad w|_{x=+\infty} = 0,$$

$$w(x,0) = 0, \qquad w(x,1) = 0.$$

We will assume that $\varphi \in H^{-1/2}([0,1])$, so we have that $w \in H^1(\Omega)$. Our goal is to compute the Dirichlet data $w|_{x=0} \in H^{1/2}([0,1])$. We discretize (17) on a set of k straight lines parallel to the y-axis and solve the semidiscrete finite-difference equation

$$-\frac{\partial^2 w_i(y)}{\partial y^2} - \frac{1}{\hat{h}_i}\left[\frac{w_{i+1}(y) - w_i(y)}{h_i} - \frac{w_i(y) - w_{i-1}(y)}{h_{i-1}}\right] = 0 \tag{18}$$

for $i = 2, \ldots, k$ with

$$\left(\frac{w_2(y) - w_1(y)}{h_1}\right) - \hat{h}_1 \frac{\partial^2 w_1(y)}{\partial y^2} = -\varphi(y)$$

and

$$w_{k+1}(y) = 0$$

serving as the boundary conditions. Let the grid correspond to the Galerkin-Petrov formulation discussed in the previous section, where we will specify U and V later. We define a semidiscrete Galerkin-Petrov solution $w_{U,V}(x,y)$ of (17) to be in U for every fixed y, and to satisfy the exact boundary and infinity conditions from (17) and the equation

$$\langle \frac{\partial v}{\partial x}, \frac{\partial w_{U,V}}{\partial x} \rangle - \langle v, \frac{\partial^2 w_{U,V}}{\partial y^2} \rangle = v(0)\varphi(y) \tag{19}$$

for any $v \in V$, if the solution exists. (Here $\langle , \rangle$ denotes the standard $L_2[0,\infty]$ inner product.) Decomposing the solutions of (18) and (19) into their Fourier series in y,

we obtain (2) and (16), respectively, with $\lambda = (i\pi y)^2$. Hence, from Proposition 3 we have that

$$w_{U,V}(0,y) \equiv w_1(y).$$

Note that conventional polynomial-based subspaces, for example, the Laguerre functions (which, as mentioned above correspond to the standard Padé approximant with a positive b) would not yield exponential convergence of the Galerkin method for nonsmooth H^1-solutions. However, the ph-element method with optimal refinement yields $O\left(e^{-c\sqrt{k}}\right)$ error with $c > 0$ for two-dimensional problems with H^1 singularities [19]. In principle, then, we could take the Galerkin subspaces from this method and apply Corollary 1 to generate the grid for the impedance-equivalent three-point scheme.

Here we demonstrate another approach based on rational approximation theory. Recall that for this problem $l = \infty$, so

$$f(\lambda) = \lambda^{-1/2}.$$

We will estimate the finite-difference impedance error

$$\|w(0,y) - w_1(y)\|_{L_2[0,1]}$$

by minimizing

$$\lambda^{-1/2} - f_k(\lambda)$$

in the sense of some weighted L^∞ norm on $(1,\infty)$ (see [14] for details). That is, we would like to find the grid which is optimal in this sense. There is a simple solution [18] which is close to optimal. We could define the grid by the multipoint Padé approximant (9) with

$$b_i = e^{\frac{(i-1)\pi}{2\sqrt{k}}},$$

so the corresponding U and V will be as in Proposition 3. From Newman's min-max estimate (well known in rational approximation theory [18]) it follows that the grid based on this multipoint Padé approximant yields for $w(x,y) \in H^1(\Omega)$,

$$\|w(0,y) - w_1(y)\|_{L_2[0,1]} = O\left(e^{-5\sqrt{k}}\right) \tag{20}$$

(see [14]). The actual computational results seem to be even better (see [2] for a numerical example where the solution belongs only to $H^{1-\epsilon}(\Omega)$, yet the convergence is asymptotically faster than the estimate (20)). It is also interesting to note here that the grid happens to be very close to the geometric progression

$$h_i = e^{\frac{(i-k)\pi}{\sqrt{k}}}, \qquad i = 1, \dots, k,$$

$$\hat{h}_1 = h_1 / \left(1 + e^{\frac{\pi}{2\sqrt{k}}}\right),$$

and

$$\hat{h}_i = \sqrt{h_{i-1} h_i}, \qquad i = 2, \dots, k.$$

See [14] for more details and results about the locations of these optimal grid points.

The optimal geometric grid described here is derived only for H^1 solutions of the Laplace equation, but it can be useful for some elliptic equations and systems with variable coefficients and singular solutions. This is because significant parts of the singularities are solutions of Laplace's equation. For example, scientists at

the international oil services company, Schlumberger, applied this optimal grid to a three-dimensional Maxwell system in inhomogeneous anisotropic media (induction logging problem). The size of the finite-difference scheme was dramatically reduced compared to the ad hoc grids used previously.

6.2. **The wave equation.** Let us now consider the initial value problem for the one-dimensional wave equation on $[0,l]\times[0,T]$,

$$\frac{\partial^2 u(x,t)}{\partial t^2}-\frac{\partial^2 u(x,t)}{\partial x^2}=0 \tag{21}$$

with boundary conditions

$$\left.\frac{\partial u}{\partial x}\right|_{x=0}=-\varphi(t),\quad u(l,t)=0,$$

$$u(x,0)=0,\quad \left.\frac{\partial w}{\partial t}\right|_{t=0}=0.$$

One may approximate u by the method of lines

$$\frac{d^2 w_i(t)}{dt^2}-\frac{1}{\hat{h}_i}\left[\frac{w_{i+1}(t)-w_i(t)}{h_i}-\frac{w_i(t)-w_{i-1}(t)}{h_{i-1}}\right]=0 \tag{22}$$

for $i=2,\dots,k$ with the boundary conditions

$$\frac{w_2(t)-w_1(t)}{h_1}-\frac{d^2 w_1(t)}{dt^2}\hat{h}_1=-\varphi(t),$$

$$w_{k+1}(t)=0,$$

$$w_i(0)=0,\quad \left.\frac{dw_i}{dt}\right|_{t=0}=0,$$

where the spatial grid is computed according to one of the Padé methods considered above. For example, let this grid correspond to the Galerkin-Petrov formulation discussed in the previous section. Define the the semidiscrete Galerkin-Petrov solution $u_{U,V}(x,t)$ of (21) to be in U for every fixed t, to have the same initial condition as u, and to satisfy the equation

$$\langle\frac{\partial v}{\partial x},\frac{\partial u_{U,V}}{\partial x}\rangle+\langle v,\frac{\partial^2 u_{U,V}}{\partial t^2}\rangle=\varphi(t)v(0) \tag{23}$$

for any $v\in V$, assuming such a solution exists. (Here $\langle,\rangle$ denotes the standard $L^2(0,1)$ inner product.) Equations (22) and (23) can be Fourier transformed to (2) and (16), respectively, so from Proposition 3 we obtain that

$$u_{U,V}(0,t)\equiv w_1(t).$$

For good subspaces, e.g., polynomial, and regular enough $\varphi(t)$, the Galerkin-Petrov solution converges exponentially; therefore, the component $w_1(t)$ of the semidiscrete finite-difference solution also converges exponentially.

Let us consider a numerical example which was given in [2] for the problem (21) where

$$\Omega=[0,1]\times[0,5]$$

with

$$\varphi=-\frac{\partial g(t)}{\partial t},$$

where $g(t)$ is a wavelet which is close to the Gaussian pulse

$$e^{-27(t-0.225)^2}.$$

The exact solution of this problem is

$$u = g(x-t) + \sum_{i=1}^{\infty}(-1)^i[g(x-t+i+1) + g(x+t-i-1)].$$

Of course, we could simply construct a grid based on the Galerkin polynomial method from Proposition 2. This would be much better than a standard equidistant grid, but we could use the available information about the solution even more efficiently. We can map (21) to (1) by a Fourier transform. Applying the same transform to the wavelet $g(\lambda)$, we find that the spectrum lies mainly in $[-8100, 0]$, so we want to choose a grid with the best approximating properties for λ from that interval. The eigenvalues of (1), i.e., the poles of f, are given by

$$\omega_i = -[\pi(i-1/2)]^2.$$

Note that the first 28 of them are located in our approximation interval, and this complicates the implimentation of the multipoint Padé approximant. In all previous discussions we wanted to approximate f for λ away from its poles.

To circumvent this problem, we use the algorithm proposed in [9]. That is, first we exactly match those poles as in (7). Next we use the remaining degrees of freedom to match the impedance at points b_i located close to the roots of a

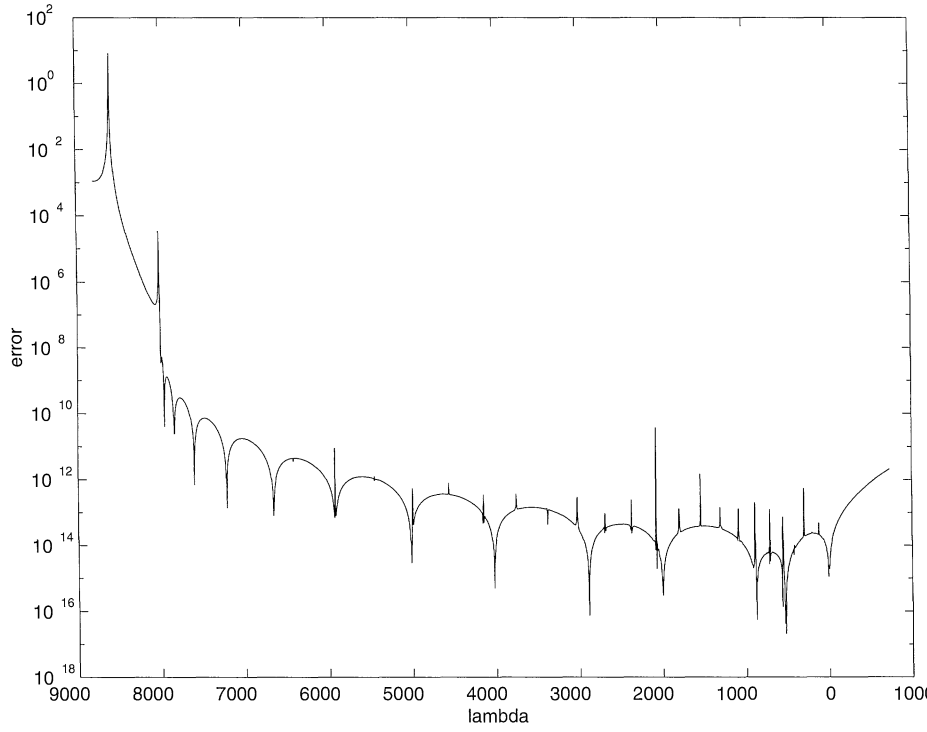

FIGURE 1. The finite-difference impedance error.

FIGURE 2. Grid, $k = 35$, "dots" are x_i, "crosses" are $\hat{x}_i$.

Chebyshev polynomial. We can then combine Propositions 1 and 3 to obtain the equivalent Galerkin-Petrov subspaces. So in addition to

$$u(x)|_{\lambda=b_i},$$

the subspaces consist of the eigenfunctions

$$\cos[\pi(i-1/2)x]$$

corresponding to the exactly matched poles. Similar combined subspaces have been used in the framework of the conventional spectral method (see for example [6]). Thus, the size k of the grid should at least be equal to the number of those poles which lie in the spectral interval which we would like to approximate. This corresponds to the famous Nyquist (lower) limit of two points per minimal wavelength for spectral methods.

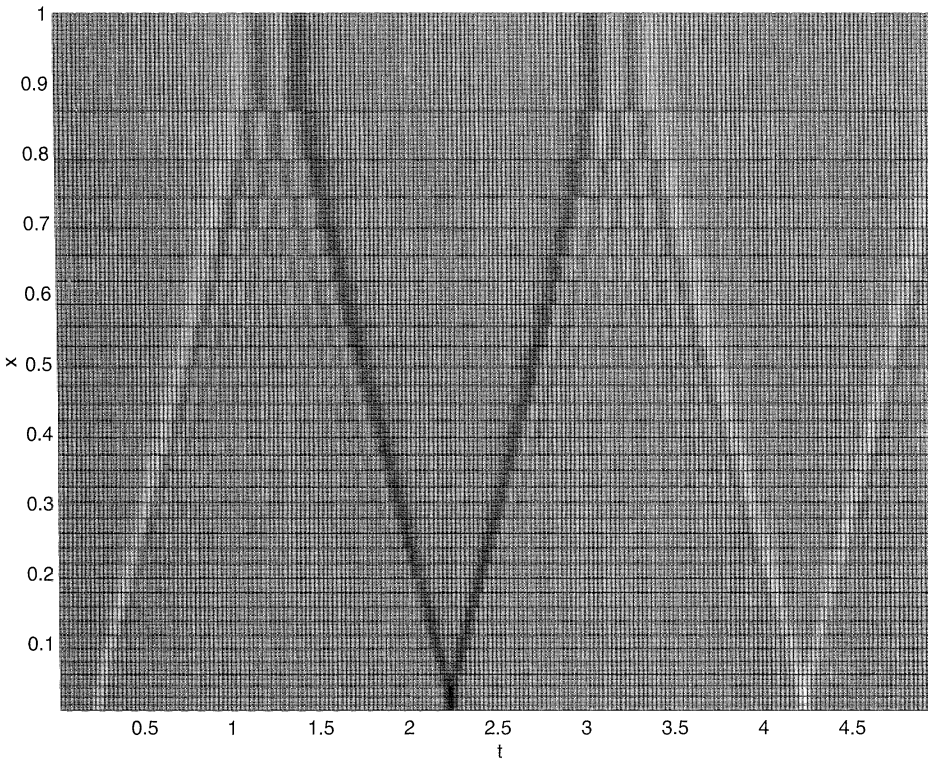

FIGURE 3. The optimal grid finite-difference solution in $x-t$ coordinates. After every reflection the numerical dispersion is reversed.

In Figure 1, we considered a grid with $k = 35$, and plotted the absolute value of the impedance error $f - f_k$ as a function of λ. The lower spikes of the curve correspond to the points b_i for which the impedance was matched exactly. The upper spikes indicate the locations of the the matched poles ω_i. As we see, the approximation error is very small within the targeted spectral interval. The grid is shown in Figure 2. Note its staggeredness (potential and derivative points alternate), which was not imposed a priori on the grid generation algorithm. Note also the gradual refinement toward $x = 0$, which is similar, but not exactly equal to, the Legendre-Gauss-Lobatto points. The grid has about 2.5 grid points per minimal wavelength of the signal on average, but some steps are larger by far than the wavelet size. According to the numerical experiments presented in [2, Table 1], the minimal grid steps (and so the stability CFL conditions) for such grids are just insignificantly smaller (about 10%) than the step size of the equidistant grid which has the same approximation error.

We computed a finite-difference solution of this hyperbolic problem by using the standard explicit FDTD with equal time steps. A two-dimensional plot of the finite-difference solution $\hat{u}$ is presented in Figure 3. Due to the grid coarsening, the wavelet becomes greatly distorted when it moves away from $x = 0$, but the distortion is almost completely reversed when the wave moves back after it hits the opposite boundary. Such behaviour is counterintuitive because usually the finite-difference errors of hyperbolic equations propagate along characteristics. However, our finite-difference solution at $x = 0$ (and only at that point) is equivalent to the Galerkin-Petrov solution on well-chosen trigonometric subspaces. This is why we do

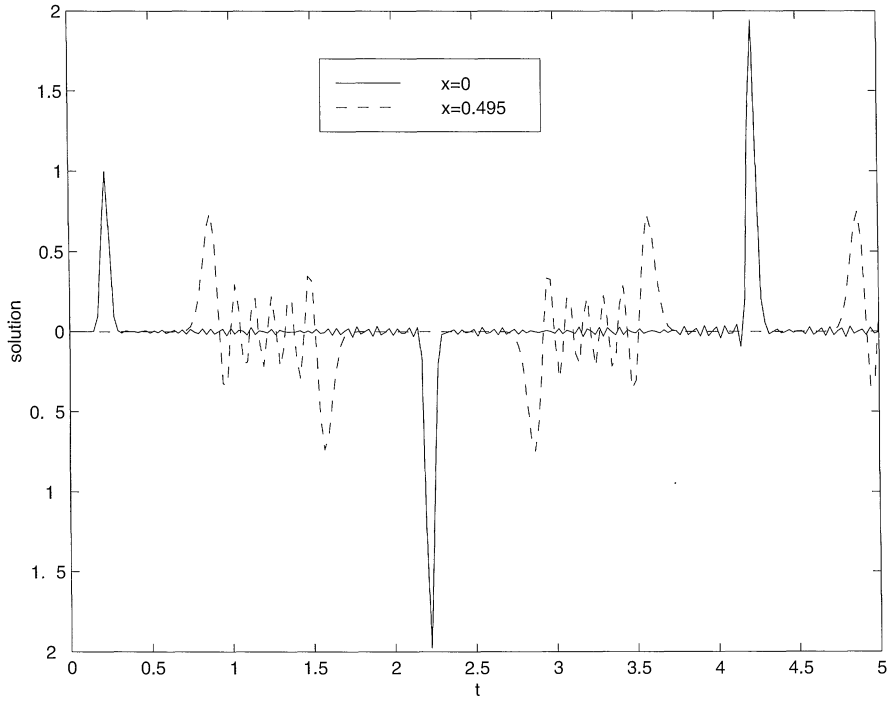

FIGURE 4. The finite-difference solution at $x = 0$ compared to x in the center of the interval.

not observe a finite-difference dispersion error at that point. We should point out that the grid constructed from a Galerkin polynomial method (i.e., simple Padé) would give qualitatively similar results but would require about twice as many grid points for the same accuracy. We plotted separately the slices of the finite-difference solution at the targeted boundary and at the center of the interval in Figure 4.

The numerical dispersion at the target does not exceed 1%. The finite-difference solution here almost exactly coincides with the properly shifted and superimposed wavelet. However, the error at the center of the spatial interval is larger than 50% of the maximal signal and greatly distorts the shape of the wavelet.

Finally, for comparison, we add to the optimal grid one potential node and one derivative node at the points $(x_{34} + x_{35})/2$ and $(\hat{x}_{34} + \hat{x}_{35})/2$, respectively. This halves the maximal grid step and apparently the local finite-difference truncation error. One would expect that this would decrease the numerical dispersion, but according to Figure 5 this is not the case. Apparently, these additional nodes destroy the delicate equivalence of the finite-difference scheme to the Galerkin-Petrov approximation. We should point out, however, that adding or deleting nodes in close proximity to the origin does not affect the accuracy so much. A theoretical analysis of the grid sensitivity could be an interesting topic for future research.

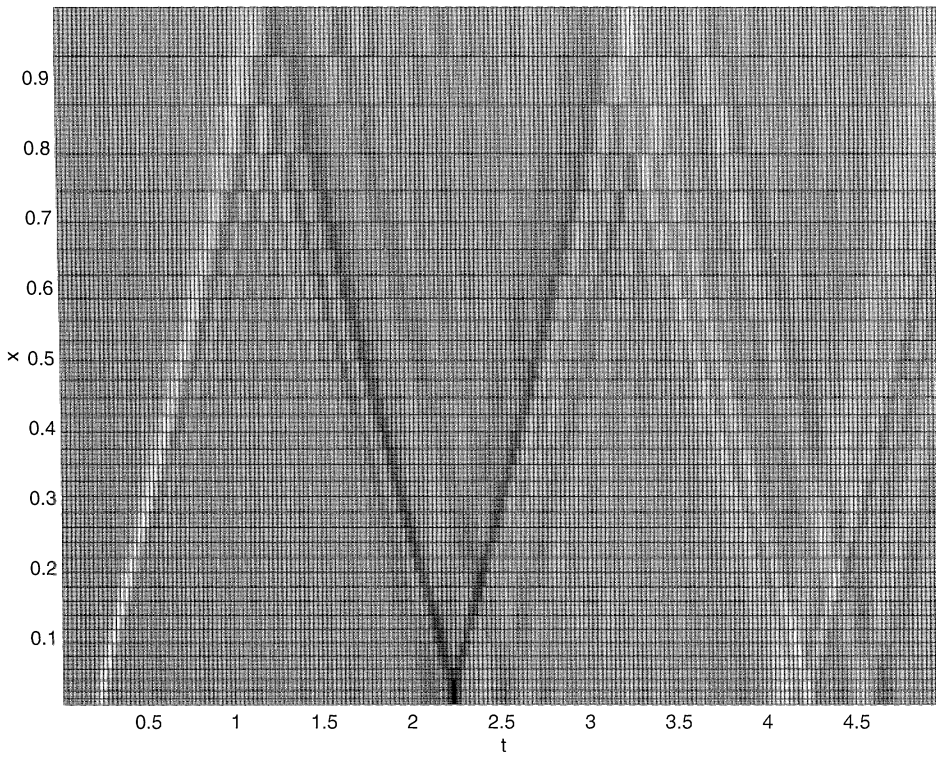

FIGURE 5. The finite-difference solution in $x - t$ coordinates, the optimal grid unbalanced by additional nodes. The numerical dispersion grows monotonically with time.

6.3. **Discretization in two dimensions.** In higher-dimensional problems for which the domain can be partitioned into rectangular subdomains, (such that within every subdomain the variables can be separated), one can apply this optimal grid method. In [9] the authors implemented this approach and observed exponential convergence at the subdomain corners. Here we give an example of a two-dimensional problem on one rectangle, and show that the method is equivalent to a spectral Galerkin method at one corner. We must remark, though, that the following example is not scientifically interesting in itself since the true solution is undefined at this corner where the two methods give the same value. However, the result found here shows equivalence for more interesting time dependent problems. Also it will provide a theoretical basis for the multidomain two-dimensional applications we discuss in [10].

Consider the Helmholtz problem where the domain

$$\Omega = (0,1) \times (0,1)$$

with

$$\partial\Omega_1 = \partial\Omega \cap (\{x_1 = 0\} \cup \{x_2 = 0\}),$$

$$\partial\Omega_2 = \partial\Omega \cap (\{x_1 = 1\} \cup \{x_2 = 1\}),$$

and u is the solution to

$$\Delta u - \lambda u = 0 \quad \text{on } \Omega,$$

$$\frac{\partial u}{\partial n} = \delta_{(0,0)} \quad \text{on } \partial\Omega_1,$$

$$u = 0 \quad \text{on } \partial\Omega_2,$$

where $\delta_{(0,0)}$ is the Dirac delta function at the origin, i.e., we consider the problem with a point source at the corner. Note that the solution u is infinite at the origin, but our goal at the moment is to show equivalence of two methods at this corner, not to prove convergence of either. Let us first describe the optimal grid finite-difference approach to this problem. We use the simple Padé approximant (8) to compute a one-dimensional optimal grid for the problem

$$P'' - \lambda P = 0, \tag{24}$$

$$-P'(0) = 1,$$

$$P(1) = 0,$$

for some b outside the spectrum (note that this is the same as (1)). That is, the one-dimensional difference solution $\tilde{P}$ would satisfy

$$L_h\tilde{P} - \lambda\tilde{P} = -\frac{1}{\hat{h}_1}e_1,$$

where e_1 is the unit vector with support in the first component. Next we take the tensor product of this grid with itself to obtain a two-dimensional Cartesian grid

on Ω, and solve the five-point difference problem

$$\begin{aligned}(25)\qquad &\frac{1}{\hat{h}_i}\left(\frac{w_{i+1,j}-w_{i,j}}{h_i}-\frac{w_{i,j}-w_{i-1,j}}{h_{i-1}}\right)\\ &+\frac{1}{\hat{h}_j}\left(\frac{w_{i,j+1}-w_{i,j}}{h_j}-\frac{w_{i,j}-w_{i,j-1}}{h_{j-1}}\right)-\lambda w_{i,j}=0\\ &\text{for } i,j=1,\dots,k\end{aligned}$$

with boundary conditions

$$w_{i,k+1}=0, \qquad w_{k+1,j}=0$$

and

$$-\frac{w_{1,j}-w_{0,j}}{h_0}=\frac{\delta_{1j}}{\hat{h}_1}, \qquad -\frac{w_{i,1}-w_{i,0}}{h_0}=\frac{\delta_{1i}}{\hat{h}_1}.$$

In short, the difference equation for w would be

$$(26)\qquad (M_h-\lambda)w=-\frac{1}{\hat{h}_1^2}e_1\otimes e_1,$$

where M_h is defined on tensor products of vectors by

$$M_h(x\otimes y)=(L_hx)\otimes y+x\otimes(L_hy).$$

Define the discrete impedance function from this difference method by

$$(27)\qquad F_k(\lambda)\equiv w_{1,1}.$$

We will need the following lemma which says that this difference equation is separable in the same way as the differential equation.

Lemma 5. *Let z_m,θ_m and z_n,θ_n be eigenpairs of the one-dimensional difference operator L_h. Then the tensor product of these vectors*

$$(z_{mn})_{ij}=(z_m)_i\,(z_n)_j$$

is an eigenvector of the two-dimensional difference operator M_h with eigenvalue

$$\theta_{mn}=\theta_m+\theta_n.$$

The proof of this lemma follows immediately by substituting z_{mn} into (25).

Now consider a variational approach to this problem. Define the energy inner product

$$E_\lambda(u,v)=\int_\Omega \nabla u\cdot\nabla v+\lambda\int_\Omega uv$$

so that the true solution u solves

$$E_\lambda(u,v)=v(0,0)$$

for any smooth v. For a finite dimensional space U, define the Galerkin solution to be $u_U\in U$ such that

$$E_\lambda(u_U,v)=v(0,0)$$

for any $v\in U$, with the corresponding impedance approximation

$$F_U\equiv u_U(0,0).$$

Let $P(x,\lambda)$ be the solution to the one-dimensional problem (24), and define

$$L = \operatorname{span}\left[\left.\frac{\partial^i}{\partial\lambda^i}P(x,\lambda)\right|_{\lambda=b} \quad i = 1\dots 2k\right].$$

We will say that $\dot{u}$ is a Galerkin eigenvector with eigenvalue μ if $\dot{u}\in U$ and

$$E_\mu(\dot{u}, v) = 0$$

for any $v \in U$.

Lemma 6. *Let $\dot{u}^m$ and $\dot{u}^n$ be L^2-normalized eigenvectors to the one-dimensional Galerkin problem with Galerkin subspace L corresponding to eigenvalues μ_m and μ_n, respectively. Then the tensor product of these vectors*

$$\dot{u}^{mn} = \dot{u}^m(x_1)\dot{u}^n(x_2)$$

is an eigenvector of the two-dimensional Galerkin problem with

$$U = L\otimes L = \operatorname{span}\left[p(x_1)q(x_2) : p,q\in L\right]$$

corresponding to the eigenvalue $\mu_{mn} = \mu_m + \mu_n$.

The proof can be obtained from direct calculations.

Proposition 4. *Let $F_k(\lambda)$ be the discrete impedance* (27) *where the one-dimensional grid was generated from* (8). *Define*

$$U = L\otimes L = \operatorname{span}\left[p(x_1)q(x_2) : p,q\in L\right].$$

If $F_U(\lambda)$ is the Galerkin impedance, then

$$F_U(\lambda) \equiv F_k(\lambda).$$

Proof. Note that M_h is symmetric with respect to the weighted inner product $\hat{h}$, that is, where the ijth component is weighted by $\hat{h}_i\hat{h}_j$. Then, by the same proof as in Lemma 1, we can write the finite-difference impedance F_k as the rational function of λ,

$$F_k(\lambda) = \sum_{m,n}\frac{(z_{mn})_{1,1}^2}{\lambda-\theta_{mn}},$$

where the z_{mn} are the $\hat{h}$-normalized eigenvectors of M_h. From Lemma 5, this is just

$$\sum_{m,n}\frac{(z_m)_1^2\,(z_n)_1^2}{\lambda-\theta_m-\theta_n},$$

where the z_i are just the $\hat{h}$-normalized one-dimensional eigenvectors. Hence

$$F_k(\lambda) = \sum_{m,n=1}^{k}\frac{y_m y_n}{\lambda-(\theta_m+\theta_n)},$$

where the y_i,θ_i are the same as in the one-dimensional impedance approximation (4). At the same time, also by the proof of Lemma 1, the Galerkin solution can

be decomposed in terms of the Galerkin eigenvectors, and the impedance can be written as

$$F_U(\lambda) = \sum_{m,n=1}^{k} \frac{\dot{u}^{mn}(0,0)^2}{\lambda - \mu_{mn}},$$

where μ_{mn} are the Galerkin eigenvalues. Thus, by Lemma 6,

$$F_U(\lambda) = \sum_{m,n} \frac{\dot{u}^{m}(0)^2 \dot{u}^{n}(0)^2}{\lambda - (\mu_m + \mu_n)}.$$

Recall that the one-dimensional Galerkin impedance can also be expressed in terms of its eigendecomposition

$$f_L(\lambda) = \sum_{i=1}^{k} \frac{\dot{u}^{i}(0)^2}{\lambda - \mu_i},$$

but Proposition 2 tells us that $f_L(\lambda)$ is exactly the same as

$$f_k(\lambda) = \sum_{i=1}^{k} \frac{y_i}{\lambda - \theta_i},$$

which implies that each

$$\dot{u}^{i}(0)^2 = y_i$$

and

$$\mu_i = \theta_i.$$

Hence,

$$F_U(\lambda) \equiv F_k(\lambda).$$

□

As we already mentioned, the example considered is not scientifically interesting in itself since the true solution of the Helmholtz equation is undefined at this corner where the two methods give the same value. However, the Helmholtz problem and its approximations can be Laplace-transformed into a three-dimensional problem and its approximations, respectively. Let it be, for example, the heat equation on

$$\Omega \times (0, T)$$

with zero initial conditions and the instantaneous point source $\delta_{(0,0)}(x)\delta_0(t)$. For positive times the solution of the latter problem exists at the corner and it is regular enough for the spectral Galerkin method. Proposition 4 would then imply spectral superconvergence of the finite-difference approximation of the heat problem at this corner for $t > 0$.

Appendix A. Postprocessing for accurate computation of the solution on the entire domain

We can use the above connection to actually transform the finite difference solution to the equivalent Galerkin-Petrov solution. This could be useful since the finite-difference solution is exponentially converging only at a priori selected points, while the variational one is converging exponentially everywhere on the computational domain.

First, let us consider the one-dimensional problem from Section 2. Let $\dot{u}_i \in U$ and $\dot{v}_i \in V$ be trial and test bi-orthonormal Galerkin-Petrov eigenvectors, respectively, i.e.,

$$\langle \dot{u}_i, \dot{v}_j \rangle_{L^2[0,1]} = \delta_{i,j}$$

and

$$\langle \dot{v}_i, \dot{u}_j \rangle_{H^1[0,1]} = \theta_i \delta_{i,j},$$

where $\delta_{i,j}$ is the Kronecker symbol. For this bi-orthogonal system to be unique, we additionally impose that

$$\dot{u}_i(0) = \dot{v}_i(0).$$

Then the corresponding impedance function $f_{V,U}$ can be written in the form (4) with

$$y_i = \dot{v}_i(0)\dot{u}_i(0).$$

Now, let $w = (w_1, \dots, w_k)$ be the finite-difference solution corresponding to $f_{V,U}$, and let

$$\{z_i\}_{i=1,\dots,k}$$

be an orthonormal set of eigenvectors of the finite-difference operator (2) with weight $\hat{h}_i$. Then the corresponding impedance $f_k = f_{U,V}$ is defined as (4) with

$$y_i = (z_i)_1^2,$$

and hence

$$(z_i)_1^2 = \dot{v}_i(0)\dot{u}_i(0).$$

Decomposing $u_{U,V}$, we obtain

$$\begin{aligned} u_{U,V}(x) &= \sum_{i=1}^{k} \dot{u}_i(x) \langle \dot{v}_i, u_{U,V} \rangle_{L^2[0,1]} \\ &= \sum_{i=1}^{k} \dot{u}_i(x)\dot{v}_i(0)(\lambda - \theta_i)^{-1} \\ &= \sum_{i=1}^{k} \dot{u}_i(x) \frac{(z_i)_1^2}{\dot{u}_i(0)} (\lambda - \theta_i)^{-1}. \end{aligned}$$

Recall that

$$\langle , \rangle_{\hat{h}}$$

is the grid Euclidean inner product with weights $\hat{h}_i$. Then, using that

$$\langle w, z_i \rangle_{\hat{h}} = (z_i)_1 (\lambda - \theta_i)^{-1},$$

we finally obtain

$$u_{U,V}(x) = \sum_{i=1}^{k} \dot{u}_i(x) \langle w, z_i \rangle_{\hat{h}}. \tag{28}$$

Formula (28) transforms the grid solution into the equivalent projection solution.

We note here that the transformation (28) is linear and does not depend on λ. That is, one may insert differential or finite-difference operators in place of λ. Hence it can be applied, for example, to the semidiscretizations discussed in Section 6.

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References

[1] N. I. Akhiezer, Theory of approximation, Dover, N.Y., 1992. MR **94b:**01041
[2] S. Asvadurov, V. Druskin, and L. Knizhnerman, *Application of the difference Gaussian rules to solution of hyperbolic problems*, J. Comp. Phys, **158**, 116-135 (2000). MR **2000j:**76109
[3] G. A. Baker and P. Graves-Morris, *Padé Approximants*, Addison-Wesley Publishing Co., London et al., 1996. MR **97h:**41001
[4] K. Black, *Spectral elements on infinite domains*, SIAM J. Sci. Comput., (1998) **19**, 5, pp. 1667–1681. CMP 98:11
[5] J. P. Boyd, *Chebyshev & Fourier spectral methods*, Springer-Verlag, 1989.
[6] E. Braverman, M. Israeli, A. Averbuch, *A fast spectral solver for a 3D Helmholtz equation*, SIAM J. Sci. Comput. 1999, **20**, No 6, pp. 2237-2260. MR **2000d:**65201
[7] V. Druskin, *Spectrally optimal finite-difference grids in unbounded domains*, Schlumberger-Doll Research, Research Note, EMG-002-97-22 (1997).
[8] V. Druskin and L. Knizhnerman, *Gaussian spectral rules for the three-point second differences: I. A two-point positive definite problem in a semiinfinite domain*, SIAM J. Numer. Anal. **37**, No 2, (1999), 403-422. MR **2000i:**65163
[9] V. Druskin and L. Knizhnerman, *Gaussian spectral rules for second order finite-difference schemes*, Mathematical journey through analysis, matrix theory, and scientific computation. Numer. Algorithms **25** (2000), 139–159. CMP 2001:11
[10] V. Druskin and S. Moskow, *Three-point finite difference schemes, Padé and the spectral Galerkin method: II. Multidomain two-dimensional impedance approximation*, in preparation.
[11] B. Fornberg *Practical guide to pseudospectral methods*, Cambridge University Press, Cambridge, UK, 1996. MR **97g:**65001
[12] A. A. Gonchar, E. A. Rakhmanov, and S. P. Suetin, *On the rate of convergence of Padé approximants of orthogonal expansions*, in Progress in Approximation Theory, A. A. Gonchar and E. B. Saff, eds., Springer-Verlag, 1992, pp. 169–190. MR **94h:**41033
[13] A. A. Gonchar, G. L. Lopes, *Markov's theorem for multipoint Padé approximants*, Mat. SSSR Sbornik, **105(147)** (1978), 512–524. 639. MR **81j:**41027
[14] D. Ingerman, V. Druskin and L. Knizhnerman, *Optimal finite-difference grids and rational approximations of square root. I. Elliptic problems*, Comm. Pure. Appl. Math., **53**, (2000), no. 8, pp. 1039-1066. MR **2001d:**65140
[15] I. S. Kac and M. G. Krein, *On the spectral functions of the string*, Amer. Math. Soc. Transl., 103 (1974), pp. 19–102. MR **48:**6969
[16] S. A. Orszag, *Spectral methods for problems in complex geometries*, J. Comp. Phys., **37** (1980), pp. 70–92. MR **83e:**65188
[17] B. N. Parlett, *The symmetric eigenvalue problem*, Prentice-Hall, SIAM, 1998. MR **99c:**65072
[18] P. Petrushev, V. Popov, *Rational approximation of real functions*, Encyclopedia of mathematics and its applications, **28**, Cambridge Univ. Press, 1987. MR **89i:**41022
[19] B. Szabó, I. Babuška, *Finite Element Analysis*, Wiley & Sons, 1991. MR **93f:**73001

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