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The complex polynomial method with a least-squares fit to boundary conditions

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ABSTRACT

We present a new application of the complex polynomial method variant of the complex variable boundary element method. Instead of fitting the boundary conditions using collocation points, we minimize the error of fit in the l_2 norm to minimize the least-squares error. This approach greatly enhances the utility and efficiency of the method, allowing us to apply the method to a variety of engineering problems.

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1. Introduction

Numerical solutions of partial differential equations (PDE) involving the Laplace or Poisson equations are important topics in engineering, physics, and applied mathematics. Some applications include heat transport, Fickian diffusion, groundwater flow, contaminant flow in groundwater, stress–strain including torsion in shafts, and electrostatics. The most popular numerical techniques used to approximate solutions to such boundary value problems of these PDE include real variable boundary element methods and the domain methods of finite-difference, finite-element methods.

The complex polynomial method (CPM) has been constrained by computational capacity and precision of both hardware and software. The method approximates solutions to boundary value problems subject to a governing PDE. Using Mathematica, a mathematical computing and programming software package enables one to solve considerably more difficult and practical problems (see [8]). Until now, the CPM has used only collocation to fit to boundary conditions, which requires an equal number of basis functions and collocation points located on the problem boundary. By using a least-squares minimization approach to satisfying boundary conditions, a greater level of computational accuracy and efficiency is obtained.

2. Background

The CPM is a numerical procedure that uses a set of complex variable monomials with complex coefficients to form a complex variable polynomial for use as an approximation function. The monomial coefficients are then determined according to the particular approach selected for satisfying the problem boundary conditions. Because complex monomials can be resolved into two real variable functions (the real and imaginary components), both parts are handled as basis functions. Hromadka and Guymon first developed the CPM variant of the complex variable boundary element method (CVBEM) and successfully applied it to a limited set of engineering problems [3]; however, the basis functions used in the CVBEM made the computations involved considerably easier, which directed further research toward the CVBEM. Details regarding earlier work with the CPM can be found in [3,8]. The CPM was recently used to solve PDE of the Laplace equation type, using Mathematica, a mathematical computation and programming software (see [8]). In [8], it is shown that complex polynomials in excess of degree 35 were computationally efficient. This computational success provided a considerable advantage over the other computer solutions applied with the CPM such as seen in [3] and has returned the CPM as being a strong topic for further research.

3. Theory

3.1. Mathematical development

Complex polynomials are entire functions, being analytic over the entire complex plane; therefore, both of the real and

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imaginary parts of the complex polynomial satisfy the Cauchy–Riemann conditions over the entire plane, resulting in both the real and imaginary parts of the complex polynomial satisfying the Laplace equation. Additionally, the real and imaginary parts of the complex function form a conjugate pair which can represent the streamline function and the associated potential function as parts of the solution to the boundary value problem.

The CPM application developed for Mathematica [8] used a collocation technique to determine the coefficients for the complex polynomial approximation function. Consequently, the coefficients were determined to match boundary condition values specified at a set of collocation points located on the problem boundary. Numerical accuracy was increased by adding more collocation points on the problem boundary and, consequently, increasing the degree of the complex polynomial.

In the current paper, the CPM is extended to using a least-squares error minimization technique in the complex polynomial approximation function matching the problem boundary conditions continuously along the entire problem boundary. With this new approach for the CPM, convergence of the CPM is guaranteed as the complex polynomial degree increases (see Theorem provided in [10]). Furthermore, the computational advantages afforded by Mathematica (and other similar software packages) still apply as reported in the collocation version of the CPM [8].

Convergence of either modeling approach can be assessed by the usual theoretical bounds (for example, see [1]) provided by the infinity-norm (with relevant assumptions made regarding gradients of boundary condition values on the problem boundary) for the point collocation approach, and by Bessel's inequality for the least-squares error minimization approach. The least-squares error minimization approach does not require assumptions to be made regarding boundary condition value gradients on the problem boundary.

A convenient approach for assessing computational accuracy is the approximate boundary approach (see [2,5]) where the locus of points where the approximation function achieves the problem boundary conditions is used to compare with the actual problem boundary. Spatial departures between the approximate boundary and the true problem boundary are reduced by adding more basis functions (higher ordered monomials) and weighting the inner product at locations of high departure by concentrating additional density of evaluation points.

The inner product formulation includes integrals as shown in Eq. (4). However, in order to evaluate these various integrals, a numerical integration is used which results in the use of an equivalent finite-dimensional vector space in $\mathbb{R}^n$ with the usual vector inner product (for example, see [1]). Generally, the numerical integration of these inner product integrals is based upon an evenly spaced set of evaluation points defined on the problem boundary that are only used as locations for evaluating the various basis functions on the problem boundary. In practice, the definitions of these evaluation points are generally not evenly spaced which results in a weighting of the inner product according to evaluation point density along the problem boundary. As the evaluation point density increases uniformly along the problem boundary, the numerical integration of the various inner product integrals becomes more accurate.

Mathematica affords the user a set of helpful procedures for numerical calculations. Extended-precision computation allows the use of almost any specified number of decimal places for the calculation at the cost of time and memory. Computation is not constrained to machine or double precision. Numerical-precision control allows the user to explicitly set the input or output precision of calculations, while numerical-precision tracking internally records the accuracy of calculated results for all computations [11].

3.2. Numerical modeling approach

Assume a simply connected domain Ω with a simple closed contour boundary Γ subject to Laplace's equation

$$\nabla^2\phi(z) = 0, \tag{1}$$

where $\phi(z)$ is the real part of a complex function $w(z) = \phi(z) + i\psi(z)$, m boundary points $z_j \in \Gamma$ are specified on Γ, and we want to determine $\hat{\phi}$, the best approximation of ϕ.

We choose a set of n monomials $\{z^0, z^1, z^2, \ldots, z^n\}$ and construct a set of global vectors, $\{\vec{F}_j\}$ to be evaluated at evaluation points (and not collocation points) simply used for locations of function evaluation such that

$$\vec{F}_j = \begin{bmatrix} f_j(z_0) \\ f_j(z_1) \\ \vdots \\ f_j(z_m) \end{bmatrix} = \begin{bmatrix} (z_0)^j \\ (z_1)^j \\ \vdots \\ (z_m)^j \end{bmatrix}. \tag{2}$$

We solve the problem in a Hilbert space using the l_2 norm and the following inner product for elements u, v:

$$\langle u, v\rangle = \int_\Gamma uv\, d\Gamma + \int_\Omega \nabla^2 u \nabla^2 v\, d\Omega = \int_\Gamma uv\, d\Gamma, \tag{3}$$

where the Laplacian operating on the elements u, v equals zero.

We orthonormalize the set of $\vec{F}_j$ vectors using the Gram–Schmidt procedure, which yields the set of orthonormalized vectors $\{\vec{G}_j\}$. We then approximate ϕ as

$$\hat{\phi}(z) = Re\left[\sum_{m=1}^{n} \lambda_j g_j\right], \tag{4}$$

where each λ_j is a unique complex constant and g_j are the basis functions which comprise $\{\vec{G}_j\}$.

We want to find the $\hat{\phi}$ which minimizes the l_2 norm on the problem boundary, Γ,

$$\|\hat{\phi} - \phi\|_2. \tag{5}$$

The defined error is a minimum when the coefficients, λ_j, equal the generalized Fourier coefficients. Through a back-substitution routine, we calculate the coefficients, c_j, corresponding to the complex monomials to substitute into our approximate solution,

$$\hat{\phi} = Re\left[\sum_{m=1}^{n} c_j z^j\right] \tag{6}$$

which best approximates ϕ on Γ in a least-squares sense.

4. Application

As part of this research, the new variant of the CPM was applied to a variety of engineering problems. We only present an application to torsion in a cylindrical shaft as a demonstration.

4.1. Torsion in a cylindrical shaft

A common problem in engineering applications and design is the analysis of stress in a shaft under rotational torsion. Some situations which require such an analysis include helicopter rotor shafts, ship propeller shafts, and automobile axles. The mathematical description of such stress is given by the Poisson equation, $\nabla^2\phi = -2$ (for example, see [6]).

In the current application, stress in a circular cross section is modeled using the CPM variant of the CVBEM. The CPM approach to this problem is to determine a particular solution to the governing PDE, ϕ_p, and then subtract the function ϕ_p from the

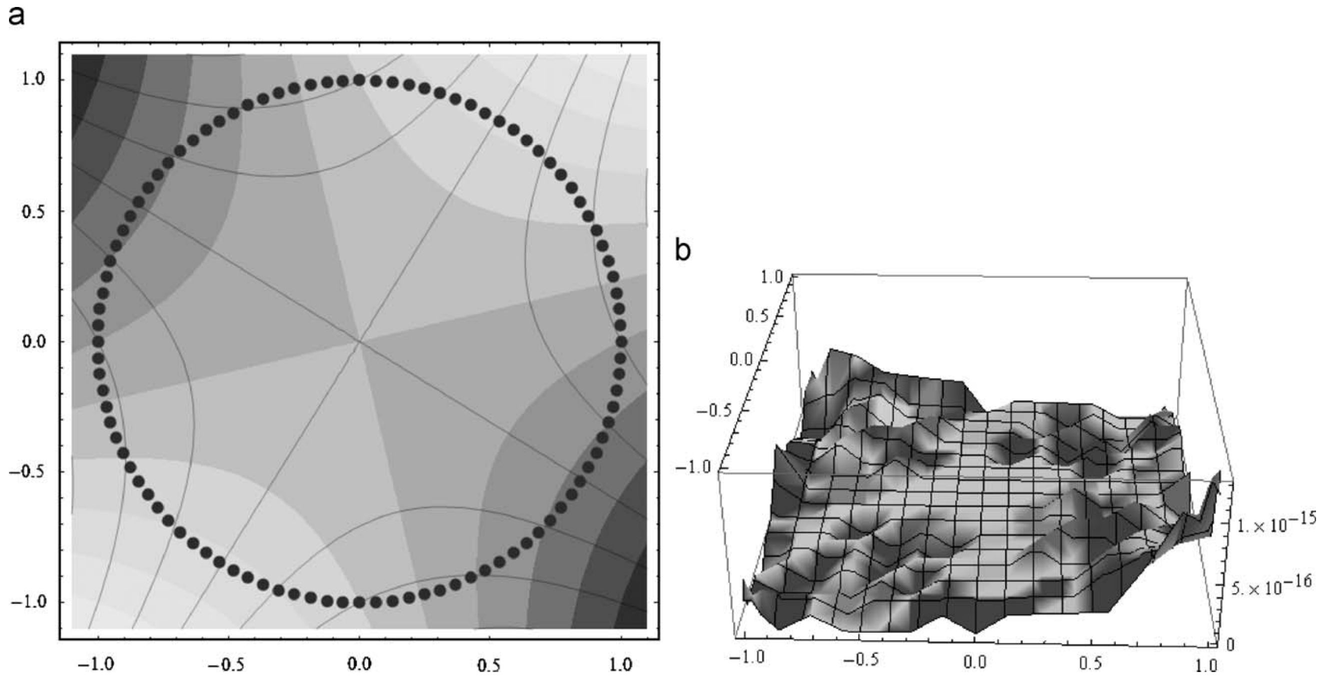

Fig. 1. Approximate solutions for $f(z) = -x^2 + 2xy + 5$, torsion in a cylindrical shaft. (a) Approximate solution. (b) Relative error.

problem boundary condition values to obtain a displaced set of boundary conditions for direct use in solving a standard two-dimensional Laplace equation problem by the CPM. The numerical solution is completed by adding the resulting CPM polynomial approximation of the Laplace equation problem to the particular solution [7]. In the application, we use a complex polynomial of degree 12 to achieve relative error on the order of 10^{-16} (Fig. 1(b)).

5. Conclusions

The CPM is extended from the collocation approach presented in [7] to a least-squares error minimization approach where the difference between approximation and measured boundary values is minimized continuously along the problem boundary using a Gram–Schmidt procedure. This new version of the CPM is developed using Mathematica although other programs such as Maple and MATLAB are available for use. The CPM and CVBEM have an advantage over finite-element and finite-difference methods because they exactly solve the governing PDE over the problem domain.

By using the Bessel's inequality,

$$\int_{\Omega \cup \Gamma} \phi^2 \geqslant \sum_{j=1}^{\infty} (\lambda_j)^2 \tag{7}$$

which bounds the approximate solution, we can measure the rate of convergence for the modeling routine. Increasing the number of basis functions will improve the fit.

The extensions of the CPM to the use of other types of boundary conditions, such as gradients tangential or normal to the problem boundary, can be readily accommodated by use of the relevant spatial gradients of the complex monomials. Such an approach is examined for use of other basis function types such as complex logarithm and products of complex logarithms with complex polynomials in other works (for example, see [2,5]).

Complex monomials are used as basis functions here; however, any set of linearly independent functions can be used. Future work will use CVBEM basis functions in order to compare the results with complex polynomial basis functions and direct further work.

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Appendix A. Mathematica program

Contact the lead author to obtain a copy of the developed computer code.

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