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# 1 Problems Studied

The primary focus of this project was on the analysis and development of new parallel algorithms for the solution of linear and nonlinear initial/boundary value problems (IBVPs) in two space variables. Parabolic, second order hyperbolic, biharmonic, and Schrödinger-type problems were considered. The new algorithms, which are alternating direction implicit (ADI) orthogonal spline collocation (OSC) methods employing  $C^1$  piecewise polynomial spaces of arbitrary order, have been implemented and their efficacy was demonstrated on test problems taken from the literature. Rigorous stability and convergence analyses of the methods were also carried out.

## 2 Summary of Results

### 2.1 Parabolic IBVPs

In [3], an ADI Crank-Nicolson scheme is considered for the solution of the linear parabolic initial-boundary value problem

$$\begin{aligned}\frac{\partial u}{\partial t} + (L_1 + L_2)u &= f(x, y, t), & (x, y, t) \in \Omega_T, \\ u(x, y, 0) &= g_1(x, y), & (x, y) \in \Omega, \\ u(x, y, t) &= g_2(x, y, t), & (x, y, t) \in \partial\Omega_T,\end{aligned}$$

where, here and in what follows,

$$\Omega = (0, 1) \times (0, 1), \quad \Omega_T = \Omega \times (0, T], \quad \partial\Omega_T = \partial\Omega \times (0, T],$$

and the linear differential operators  $L_1$  and  $L_2$  are given by

$$(1) \quad L_1 u = -a_1(x, y, t) \frac{\partial^2 u}{\partial x^2} + b_1(x, y, t) \frac{\partial u}{\partial x} + c(x, y, t)u, \quad L_2 u = -a_2(x, y, t) \frac{\partial^2 u}{\partial y^2} + b_2(x, y, t) \frac{\partial u}{\partial y}.$$

In comparison to the scheme outlined in the original proposal, the new ADI scheme uses  $L_2^{n+1/2}$  in place of  $L_2^n$  and  $L_2^{n+1}$ . Using a new approach, we show that the scheme is second-order accurate in time and of optimal third-order accuracy in space in the  $H^1$  norm. For simplicity, the analysis in [3] is presented for the case of a spatial discretization based on piecewise Hermite bicubics, but is easily extended to OSC discretization with piecewise polynomials of higher degree. We also give a new efficient implementation of the scheme and test it on a sample problem for accuracy and convergence rates in various norms. Earlier implementations of ADI OSC schemes were based on determining, at each time level, a two-dimensional approximation defined on  $\Omega$ . In the new implementation, at each time level, we determine one-dimensional approximations along horizontal and vertical lines passing through Gauss points and obtain the two-dimensional approximation on  $\Omega$  at the final time level corresponding to  $t = T$ . It should be noted that with respect to the implementation of OSC schemes the non-divergence forms of  $L_1$  and  $L_2$  in (1) are more natural than the divergence forms of  $L_1$  and  $L_2$  which are typically used in finite element (FE) spatial discretization. In fact, ADI FE Galerkin methods for solving variable coefficient parabolic problems in the divergence form were considered in [7]. However, our two-level, parameter free ADI OSC scheme does not have a FE Galerkin counterpart. The method of [7] of comparable accuracy is the three level ADI Laplace-modified scheme requiring the selection of a stability parameter. Our ADI OSC scheme

with piecewise polynomials of degree  $\geq 3$  is more accurate than the standard ADI finite difference scheme which is only second-order accurate in both time and space.

In [4], we consider a nonlinear parabolic initial-boundary value problem on a rectangular polygon with the solution satisfying variable coefficient Robin's boundary conditions. An approximation to the solution at a desired time value is obtained using an alternating-direction implicit extrapolated Crank-Nicolson scheme in which orthogonal spline collocation with piecewise polynomials of an arbitrary degree  $\geq 3$  is used for spatial discretization. For rectangular and  $L$  shaped regions we describe an efficient  $B$ -spline implementation of the scheme and present numerical results demonstrating the accuracy and convergence rates in various norms. For problems with homogeneous Dirichlet boundary conditions, we observe a superconvergence phenomenon when the initial condition is approximated using the Gauss interpolant rather than the quasi-interpolant suggested in [8] for parabolic equations in a single space variable.

In the special case in which the region is a square and Dirichlet boundary conditions are prescribed, the problem considered in [4] is of the form

$$\frac{\partial u}{\partial t} - a_1(x, y, t, u, \nabla u) \frac{\partial^2 u}{\partial x^2} - a_2(x, y, t, u, \nabla u) \frac{\partial^2 u}{\partial y^2} = f(x, y, t, u, \nabla u), \quad (x, y, t) \in \Omega_T,$$

$$u(x, y, 0) = g_1(x, y), \quad (x, y) \in \Omega,$$

$$u(x, y, t) = g_2(x, y, t), \quad (x, y, t) \in \partial\Omega_T.$$

We have carried out convergence analysis for the case in which the right hand side  $f$  depends on  $u$  and  $\nabla u$  but the coefficients  $a_1$  and  $a_2$  are independent of these quantities. We expect to extend our analysis to the case in which  $a_1$  and  $a_2$  depend on  $u$  using new results obtained by our graduate student Abdulrahim Aitbayev who in his Ph.D. dissertation [1] obtained new convergence results for the OSC solution of the nonlinear elliptic boundary value problem

$$a_{11}(x, y, u, \nabla u) \frac{\partial^2 u}{\partial x^2} + a_{12}(x, y, u, \nabla u) \frac{\partial^2 u}{\partial x \partial y} + a_{22}(x, y, u, \nabla u) \frac{\partial^2 u}{\partial y^2} + c(x, y, u, \nabla u) = f(x, y), \quad (x, y) \in \Omega,$$

$$u(x, y) = 0, \quad (x, y) \in \partial\Omega.$$

## 2.2 Hyperbolic IBVPs

In [14], two schemes are formulated and analyzed for the approximate solution of the linear second order hyperbolic problem

$$\frac{\partial^2 u}{\partial t^2} + Lu = f(x, y, t), \quad (x, y, t) \in \Omega_T,$$

$$(2) \quad u(x, y, 0) = g_0(x, y), \quad \frac{\partial u}{\partial t}(x, y, 0) = g_1(x, y), \quad (x, y) \in \Omega,$$

$$u(x, y, t) = g_2(x, y, t), \quad (x, y, t) \in \partial\Omega_T,$$

where the linear differential operator  $L$  is given by

$$Lu = -\frac{\partial}{\partial x} \left( a_1(x, y, t) \frac{\partial u}{\partial x} \right) - \frac{\partial}{\partial y} \left( a_2(x, y, t) \frac{\partial u}{\partial y} \right) + b_1(x, y, t) \frac{\partial u}{\partial x} + b_2(x, y, t) \frac{\partial u}{\partial y} + c(x, y, t)u.$$

OSC with piecewise Hermite bicubics is used for the spatial discretization. The resulting system of ordinary differential equations in the time variable is discretized using perturbations of standard finite difference approximation procedures to produce Laplace-modified (LM) and ADI schemes. It is shown that the OSC LM and ADI schemes are unconditionally stable and of optimal order accuracy in the  $H^1$  and discrete maximum norms for the space and time variables, respectively, provided a stability parameter, which appears in all LM type methods, is chosen appropriately. In the convergence analysis, a bicubic interpolant of the solution  $u$  of (2) is used as a comparison function. The algebraic problems to which these schemes lead are also described and numerical results are presented for an implementation of the OSC ADI scheme to demonstrate the accuracy and rate of convergence of the method.

In [5], we consider the approximate solution of the linear second order hyperbolic problem

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} + (L_1 + L_2)u &= f(x, y, t), \quad (x, y, t) \in \Omega_T, \\ u(x, y, 0) &= g_0(x, y), \quad \frac{\partial u}{\partial t}(x, y, 0) = g_1(x, y), \quad (x, y) \in \Omega, \\ u(x, y, t) &= g_2(x, y, t), \quad (x, y, t) \in \partial\Omega_T, \end{aligned}$$

where the linear differential operators  $L_1$  and  $L_2$  are given by (1). With  $\mathcal{G}$  the set of Gauss points in  $\Omega$ ,  $\tau = T/M$ , and  $t_n = n\tau$ , the new OSC ADI scheme consists in finding piecewise Hermite bicubics  $u_h^n$ ,  $n = 2, \dots, M$ , such that for  $n = 1, \dots, M - 1$ ,

$$\begin{aligned} (3) \quad (I + 0.5\tau^2 L_1^n) \tilde{u}_h^n(\xi) &= f(\xi, t_n) + 2\tau^{-2} u_h^n(\xi), \quad \xi \in \mathcal{G}, \\ (I + 0.5\tau^2 L_2^n)(u_h^{n+1} + u_h^{n-1})(\xi) &= \tau^2 \tilde{u}_h^n(\xi), \quad \xi \in \mathcal{G}, \end{aligned}$$

where  $u_h^0, u_h^1, u_h^n|_{\partial\Omega}$ ,  $n = 2, \dots, M$ , are assumed to be given, and where  $L_1^n, L_2^n$  are the differential operators of (1) with  $t = t_n$ . In the first equation of (3), for each Gauss point  $\xi^y$  in the  $y$ -direction,  $\tilde{u}_h^n(\cdot, \xi^y)$ ,  $n = 1, \dots, M - 1$ , is a piecewise Hermite cubic in the  $x$ -direction satisfying

$$\tilde{u}_h^n(\alpha, \xi^y) = \tau^{-2}(I + 0.5\tau^2 L_2^n)(u_h^{n+1} + u_h^{n-1})(\alpha, \xi^y), \quad \alpha = 0, 1.$$

We show in [5] that the scheme (3) is second order accurate in time and of third-order accuracy in space in the  $H^1$  norm. An efficient implementation of the scheme is similar to that for the scheme of [3] and it involves representing  $u_h^n$  in terms of basis functions with respect to  $y$  alone while  $\tilde{u}_h^n$  is represented in terms of basis functions with respect to  $x$  only. It is interesting to note that for variable coefficient hyperbolic problems our parameter free ADI OSC scheme (3) does not have a finite element Galerkin counterpart.

### 2.3 Biharmonic Problems

Our graduate student, Lou Zhuoming, completed his Ph.D. dissertation and graduated in May 1996. His research was concerned with the derivation of existence, uniqueness and convergence results for OSC methods and the implementation of these methods for the solution of three biharmonic problems, based on the splitting principle [15]. The first problem comprises the biharmonic equation in  $\Omega$  with  $u = g_1$  and  $\Delta u = g_2$  on  $\partial\Omega$ . This problem becomes one of solving two nonhomogeneous Dirichlet problems for Poisson's equation. The resulting linear systems can be solved effectively with cost  $O(N^2 \log_2 N)$  using the matrix decomposition algorithm of [6]. In this case, optimal order

$H^k$ -norm error estimates,  $k = 0, 1, 2$ , are derived. In the second problem, the boundary condition on the horizontal sides of  $\partial\Omega$ ,  $\Delta u = g_2$ , is replaced by the condition  $\partial u / \partial n = g_3$ . Optimal  $H^1$ - and  $H^2$ -norm error estimates are derived and a single series OSC Fourier method is formulated for the solution of the algebraic problem. This algorithm has cost  $O(N^2 \log_2 N)$ . The third problem is the biharmonic Dirichlet problem

$$\begin{aligned} \Delta^2 u &= f(x, y), & (x, y) \in \Omega, \\ u = g_1(x, y), & \quad \frac{\partial u}{\partial n} = g_2(x, y), & (x, y) \in \partial\Omega, \end{aligned}$$

and again optimal  $H^1$ - and  $H^2$ -norm error estimates are derived. The OSC linear system is solved by a direct method which is based on the capacitance matrix technique with the second biharmonic problem as the auxiliary problem. The total cost of this capacitance matrix algorithm is  $O(N^3)$ . Results of some numerical experiments were presented which, in particular, verify the fourth order accuracy of the approximations and the superconvergence of the derivative approximations at the mesh points. The paper [16] is based on this work but uses different tools to simplify the error analyses and, in addition, answers some outstanding existence and uniqueness questions.

David Knudson completed his Ph.D. dissertation [9] and graduated in December 1997. His research was concerned with the piecewise Hermite bicubic, Ciarlet-Raviart mixed finite element Galerkin method for the solution of the biharmonic Dirichlet problem with homogeneous boundary conditions. The aim of this work was to compare the Galerkin approach with the OSC approach considered by Lou [15] and provide insight into the development of more efficient OSC methods for this problem and also certain Schrödinger systems. In [9], first existence and uniqueness of the Galerkin solution were proved. Then a Schur complement approach was used to reduce the Galerkin problem to a Schur complement system involving the approximation to  $\Delta u$  on the two vertical sides of  $\partial\Omega$  and to an auxiliary Galerkin problem for a related biharmonic problem with  $\Delta u$  instead of  $\partial u / \partial n$  specified on the two vertical sides of  $\partial\Omega$ . The Schur complement system with a symmetric and positive definite matrix was solved using the preconditioned conjugate gradient method. A preconditioner was obtained from the Galerkin problem for a related biharmonic problem with  $\Delta u$  instead of  $\partial u / \partial n$  specified on the two horizontal sides of  $\partial\Omega$ . It is conjectured that the preconditioner was spectrally equivalent to the Schur complement matrix. On an  $N \times N$  partition the cost of solving the preconditioned system and the cost of multiplying the Schur complement matrix by a vector are  $O(N^2)$  each. With the number of iterations proportional to  $\log_2 N$ , the cost of solving the Schur complement system is  $O(N^2 \log_2 N)$ . The solution to the auxiliary Galerkin problem is obtained using separation of variables and fast Fourier transforms at a cost of  $O(N^2 \log_2 N)$ . Hence the total computational cost of solving the Galerkin problem is  $O(N^2 \log_2 N)$ . Numerical results indicate that the  $L^2$  and  $H^1$  norm errors in the approximations to  $u$  and  $\Delta u$  are of optimal fourth and third orders respectively. Convergence at the nodes is fourth order for the approximations to  $u$  and  $\Delta u$  and third order for the approximations to the first order derivatives of  $u$  and  $\Delta u$ . A paper based on this research is being prepared for publication.

In [16], the linear system corresponding to the piecewise Hermite bicubic OSC solution of the biharmonic Dirichlet problem was solved using a capacitance matrix algorithm whose cost is  $O(N^3)$ . Recently, in [2], a new algorithm of cost  $O(N^2 \log_2 N)$  was developed for solving this linear system. As in [9], the algorithm of [2] involves fast Fourier transforms and solving a Schur complement linear system using the preconditioned conjugate gradient method.

## 2.4 Schrödinger Systems

In [11], Crank-Nicolson and ADI OSC schemes are formulated and analyzed for the approximate solution of the linear Schrödinger problem

$$\begin{aligned} & \frac{\partial \psi}{\partial t} - i\Delta\psi + i\sigma(x, y, t)\psi = f(x, y, t), \quad (x, y, t) \in \Omega_T, \\ (4) \quad & \psi(x, y, t) = 0, \quad (x, y, t) \in \partial\Omega_T, \\ & \psi(x, y, 0) = \psi^0(x, y), \quad (x, y) \in \Omega, \end{aligned}$$

where  $i^2 = -1$ ,  $\Delta$  is the Laplacian and  $\sigma$  is a prescribed, real function, while  $\psi$ ,  $\psi^0$  and  $f$  are complex-valued. This type of problem arises in many disciplines, such as quantum mechanics, underwater acoustics, plasma physics and seismology. Usually  $f = 0$  in quantum mechanics. We write  $\psi$ ,  $f$  and  $\psi^0$  as  $\psi_1 + i\psi_2$ ,  $f_1 + if_2$  and  $\psi_1^0 + i\psi_2^0$ , respectively. Taking real and imaginary parts of (4) then yields

$$\begin{aligned} & \frac{\partial u}{\partial t} + S(-\Delta + \sigma(x, y, t))u = F(x, y, t), \quad (x, y, t) \in \Omega_T, \\ (5) \quad & u(x, y, t) = 0, \quad (x, y, t) \in \partial\Omega_T, \\ & u(x, y, 0) = u^0(x, y), \quad (x, y) \in \Omega, \end{aligned}$$

where

$$u = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad F = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \quad \text{and} \quad u^0 = \begin{pmatrix} \psi_1^0 \\ \psi_2^0 \end{pmatrix}$$

are real-valued vector functions, and  $S$  is the  $2 \times 2$  skew-symmetric matrix

$$S = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}.$$

Hence, (5), and thus (4), is not parabolic but a Schrödinger-type system of partial differential equations. In this paper, OSC with  $C^1$  piecewise polynomials of arbitrary degree  $r \geq 3$  in each space variable is used for the spatial discretization of (5). The resulting system of ordinary differential equations in the time variable is discretized using the trapezoidal rule to produce the Crank-Nicolson OSC scheme, which is then perturbed to obtain the ADI OSC scheme. The stability of these schemes is examined and optimal order *a priori* error estimates in both the  $H^1$ -norm and the  $L^2$ -norm at each time step derived. The approach employed in the convergence analysis of the schemes is based on using, as a comparison function, a projection of the exact solution into a space of  $C^1$  piecewise polynomials of degree  $r$  in each space variable. This is a key element in the derivation of the optimal order  $L^2$ -error estimates.

In [12, 13], OSC methods are considered for the solution of problems governed by the equation

$$(6) \quad \frac{\partial^2 u}{\partial t^2} + 2\nu \frac{\partial u}{\partial t} + \Delta(q(x, y)\Delta u) = f(x, y, t), \quad (x, y, t) \in \Omega_T,$$

where  $\nu$  is a nonnegative constant related to viscous damping coefficient ( $\nu = 0$  if external viscous damping is ignored), and  $q(x, y)$  is a variable density function such that

$$0 < q_{\min} \leq q(x, y) \leq q_{\max} < \infty, \quad (x, y) \in \Omega;$$

see [10]. This equation commonly arises in plate vibration and seismological problems. The initial conditions are

$$u(x, y, 0) = g_0(x, y), \quad \frac{\partial u}{\partial t}(x, y, 0) = g_1(x, y), \quad (x, y) \in \bar{\Omega},$$

while the boundary conditions (BCs) are of one of the following three types:

BC1: "clamped" BCs:

$$u(x, y, t) = 0, \quad \frac{\partial u}{\partial n}(x, y, t) = 0, \quad (x, y, t) \in \partial\Omega_T;$$

BC2: "hinged" BCs:

$$u(x, y, t) = 0, \quad \Delta u(x, y, t) = 0, \quad (x, y, t) \in \partial\Omega_T;$$

BC3: BCs in which the vertical sides are hinged and the horizontal sides are clamped:

$$\begin{aligned} u(x, y, t) &= 0, & (x, y, t) &\in \partial\Omega_T, \\ \Delta u(x, y, t) &= 0, & (x, y, t) &\in \partial\Omega_1 \times (0, T], \\ \frac{\partial u}{\partial n}(x, y, t) &= 0, & (x, y, t) &\in \partial\Omega_2 \times (0, T], \end{aligned}$$

where

$$\partial\Omega_1 = \{(\alpha, y) : \alpha = 0, 1, 0 \leq y \leq 1\}, \quad \partial\Omega_2 = \{(x, \alpha) : 0 \leq x \leq 1, \alpha = 0, 1\}.$$

We reformulate each problem by introducing the functions

$$u_1 = e^{\nu t} \frac{\partial u}{\partial t}, \quad u_2 = q e^{\nu t} \Delta u.$$

For example, setting

$$U = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \quad F = \begin{bmatrix} e^{\nu t} f \\ 0 \end{bmatrix}, \quad G = \begin{bmatrix} g_1 \\ q \Delta g_0 \end{bmatrix},$$

in the problem with BC1, we obtain the Schrödinger system

$$\begin{cases} \frac{\partial U}{\partial t} - S_q \Delta U + \nu R U = F, & (x, y, t) \in \Omega_T, \\ U(x, y, 0) = G(x, y), & (x, y) \in \Omega, \\ u_1(x, y, t) = 0, \frac{\partial u_1}{\partial n}(x, y, t) = 0, & (x, y, t) \in \partial\Omega_T, \end{cases}$$

where

$$S_q = \begin{bmatrix} 0 & -1 \\ q & 0 \end{bmatrix}, \quad R = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Note that it is necessary to carry out an additional calculation to obtain an approximation to  $u$  from that to  $u_1$ .

To determine an approximation to  $U$ , we used OSC with  $C^1$  piecewise polynomials of arbitrary degree  $r \geq 3$  in each space variable for the spatial discretization. The resulting systems of ordinary differential equations in the time variable were then discretized using standard Crank–Nicolson or ADI techniques involving only two time levels (cf. [11]). Specifically, we formulated and analyzed

Crank–Nicolson OSC schemes for all three choices of BCs, and also formulate ADI OSC methods for BC2 and BC3 and analyzed these methods for the special case in which  $q$  is a constant and  $\nu = 0$ . Based on our experience with OSC methods for the biharmonic Dirichlet problem [16], we believe that it is not possible to formulate a standard ADI method for BC1. For this problem, we employed the capacitance matrix method (cf. [15, 16]) to solve the Crank–Nicolson scheme efficiently for the special case of constant  $q$  and  $C^1$  piecewise bicubic polynomials on a uniform partition of  $\Omega$ . We examined the existence, uniqueness and stability of each scheme and show that, for each, the  $H^m$ -norm,  $m = 1, 2$ , of the error at each time step is of optimal order  $r + 1 - m$  in space and second order in time. Implementational issues were also addressed and numerical results obtained which confirm the theoretical analyses.

### 3 Publications and Technical Reports

1. A. Aitbayev, *Orthogonal Spline Collocation for Nonlinear Elliptic Boundary Value Problems*, Ph.D. dissertation, University of Kentucky, 1998.
2. B. Bialecki, *A fast solver for the orthogonal spline collocation solution of the biharmonic Dirichlet problem on rectangles*, Numer. Math., submitted.
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## 4 Scientific Personnel

Bernard Bialecki, Graeme Fairweather, Ryan Fernandes, Abdulrahim Aitbayev, David Knudson, Bingkun Li, Zhuo-Ming Lou.

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