THE AUTOMATIC SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS USING A GLOBAL SPECTRAL METHOD

ALEX TOWNSEND* AND SHEEHAN OLVER†

Abstract. A spectral method for solving linear partial differential equations (PDEs) with variable coefficients and general boundary conditions defined on rectangular domains is described, based on separable representations of partial differential operators and the one-dimensional ultraspherical spectral method. If a partial differential operator is of splitting rank 2, such as the operator associated with Poisson or Helmholtz, the corresponding PDE is solved via a generalized Sylvester matrix equation, and a bivariate polynomial approximation of the solution of degree \((n_x, n_y)\) is computed in \(O((n_x n_y)^{3/2})\) operations. Partial differential operators of splitting rank \(\geq 3\) are solved via a linear system involving a block-banded matrix in \(O(\min(n_x^3 n_y, n_x n_y^3))\) operations. Numerical examples demonstrate the applicability of our 2D spectral method to a broad class of PDEs, which includes elliptic and dispersive time-evolution equations. The resulting PDE solver is written in MATLAB and is publicly available as part of CHEBFUN. It can resolve solutions requiring over a million degrees of freedom in under 60 seconds. An experimental implementation in the Julia language can currently perform the same solve in 10 seconds.

Key words. Chebyshev, ultraspherical, partial differential equation, spectral method

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1. Introduction. This paper describes a spectral method for the solution of linear partial differential equations (PDEs) with variable coefficients defined on bounded rectangular domains \([a, b] \times [c, d]\) that take the form:

\[ L u(x, y) = f(x, y), \quad L = \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \ell_{ij}(x, y) \frac{\partial^{i+j}}{\partial y^i \partial x^j}, \quad (1.1) \]

where \(N_x\) and \(N_y\) are the differential orders of \(L\) in the \(x\)- and \(y\)-variable, respectively, \(f(x, y)\) and \(\ell_{ij}(x, y)\) are functions defined on \([a, b] \times [c, d]\), and \(u(x, y)\) is the desired solution. The operator \(L\) is called a linear partial differential operator (PDO). Many real-world phenomena can be formalized in terms of a PDE; see, for example, [14, 15, 17].

In addition, (1.1) should be supplied with \(K_x, K_y \geq 0\) linear constraints, i.e.,

\[ \mathcal{B}_x u(x, y) = g(y), \quad \mathcal{B}_y u(x, y) = h(x), \]

to ensure that there is a unique solution. Here, \(g\) and \(h\) are vector-valued functions with \(K_x\) and \(K_y\) components and \(\mathcal{B}_x\) and \(\mathcal{B}_y\) are linear operators acting on continuous bivariate functions, which usually, but not necessarily, represent boundary conditions on the left-right and top-bottom edges of \([a, b] \times [c, d]\). For example, if \(\mathcal{B}_x\) and \(\mathcal{B}_y\) represent Dirichlet boundary conditions, then \(K_x = K_y = 2\),

\[ \mathcal{B}_x u(x, y) = \begin{pmatrix} u(a, y) \\ u(b, y) \end{pmatrix}, \quad \mathcal{B}_y u(x, y) = \begin{pmatrix} u(x, c) \\ u(x, d) \end{pmatrix}, \]

and \(g\) and \(h\) are the prescribed boundary data along the four edges. The spectral method we describe allows for general linear constraints such as Neumann and Robin

∗Department of Mathematics, Massachusetts Institute of Technology, 77 Massachusetts Avenue Cambridge, MA 02139-4307. (ajt@mit.edu)
†School of Mathematics and Statistics, The University of Sydney, Sydney, Australia. (Sheehan.Olver@sydney.edu.au)
boundary conditions, as well as the possibility of interior and integral constraints. Without loss of generality, the constraints are assumed to be linearly independent; otherwise, at least one of them can be removed while preserving the uniqueness of the solution. The existence and uniqueness of a solution to a PDE can be quite a subtle matter [26]. In this paper we always assume there is a unique solution and seek an accurate numerical approximation to it.

For integers $n_x$ and $n_y$ our spectral method returns a matrix $X \in \mathbb{C}^{n_y \times n_x}$ of bivariate Chebyshev expansion coefficients for the solution $u$ [3, Sect. 2(c)] such that

$$u(x, y) \approx \sum_{i=0}^{n_y-1} \sum_{j=0}^{n_x-1} X_{ij} T_i(y) T_j(x), \quad (x, y) \in [a, b] \times [c, d],$$

(1.2)

where $T_j(x) = \cos(j \cos^{-1} x)$ for $x \in [-1, 1]$ is the degree $j$ Chebyshev polynomial (of the first kind), and $\phi(x) = 2(x-a)/(b-a)-1$ and $\psi(y) = 2(y-c)/(d-c)-1$ are affine transformations from $[a, b]$ and $[c, d]$ to $[-1, 1]$, respectively. The approximant in (1.2) is of degree $(n_x - 1, n_y - 1)$, i.e., of degree $n_x - 1$ in $x$ and $n_y - 1$ in $y$. In practice, we adaptively determine $n_x$ and $n_y$ so that the computed bivariate polynomial in (1.2) uniformly approximates the solution on $[a, b] \times [c, d]$ to a high accuracy (see Section 5).

There are many exemplary papers that focus on solving a specific PDE and developing specialized algorithms to do so, for example, [8, 21]. In contrast, we concentrate on what can be achieved by a general solver that is merely given a description of a PDE in a syntax close to the notation found in standard textbooks [14, 15, 17]. This opens up a wonderful opportunity for a computational scientist to creatively explore and investigate in a way that can be very fruitful. As an example the following MATLAB code solves the Helmholtz equation given by $u_{xx} + u_{yy} + 1000u = \cos(10xy)$ on $[-1, 1] \times [-1, 1]$ with non-homogeneous Dirichlet conditions:

```matlab
N = chebop2(@(u) laplacian(u) + 1000*u); \% N = u_xx+u_yy+1000u
N.lbc = 1; N.rbc = 1; N.dbc = 1; N.ubc = 1; \% u=1 at boundary
f = chebfun2(@(x,y) cos(10*x.*y)); \% Construct rhs
u = N \ f; \% Solve PDE
```

The final numerical solution $u$ is represented in the MATLAB package CHEBFUN [43] (an extension of CHEBFUN [12] to bivariate functions defined on rectangles) so that we are able to conveniently perform subsequent operations on the solution such as evaluation, differentiation, and integration. CHEBFUN2 represents a function by a bivariate polynomial approximation (stored in a compressed low rank form) [43]. A chebfun (in lower case letters) is any approximant constructed by CHEBFUN2. In the Helmholtz example above the solver determines that $n_x = n_y = 257$ is sufficient to uniformly approximate the solution to 10 digits of accuracy.

While our PDE solver is relatively general, it does offer the following benefits:

- **Fast computation:** We retain the $O((n_x n_y)^{3/2})$ complexity achieved in [37] for solving Poisson and Helmholtz equations, while allowing for general linear constraints. The same complexity extends to any linear PDE associated to an operator with a splitting rank of 2 (see Section 4.3).

- **Numerical accuracy:** The final polynomial approximant usually approximates the PDE solution to an accuracy close to machine precision relative to the absolute maximum of the solution (see Section 7).

- **Spectral convergence with general linear constraints:** If the solution to a PDE is smooth, then there are many methods that achieve spectral convergence, but usually for very specific boundary conditions or require an appropriate
basis to be selected in advance [23, 37]. Here, our spectral method handles
genral linear constraints such as Dirichlet, Neumann, or Robin conditions in
an automatic manner (see Section 6) and always represents the final solution
in the tensor product Chebyshev basis.

- **Accuracy for solutions with weak singularities:** The solution to a linear PDE
  with smooth variable coefficients defined on a rectangular domain can have
  weak corner singularities (consider \(-\nabla^2 u = 1\) with homogeneous Dirichlet
  boundary conditions [7, p. 38]). To globally resolve such a solution a high
  degree bivariate polynomial approximation may be required. The solver we
  describe is fast and numerically stable so high degree approximants can be
  reliably computed to resolve solutions with weak corner singularities.

- **Automated PDE solver:** The resulting PDE solver is supplied with an anony-
  mous function handle defining a PDO together with linear constraints. The
  discretization required to resolve the solution is automatically determined.
  The solver returns an accurate polynomial approximation of the solution rep-
  resented as a chebfun2.

The original motivation for this paper was to develop a 2D analogue of the
CHEBOP system [11], which solves ordinary differential equations (ODEs) on bounded
intervals in an automated manner using an adaptive 1D spectral collocation method.
Our 2D spectral method has a different underlying methodology, but the user inter-
face closely resembles that of its predecessor. In particular, the backslash command \(x = \text{A} \backslash \text{b}\) for solving linear systems in \text{MATLAB} that is overloaded (in the computer pro-
gramming sense of the term) by CHEBOP to solve linear ODEs in [11] is now overloaded
by CHEBOP2 for linear 2D PDEs, i.e., \(u = \text{A} \backslash \text{f}\) (see the code snippet above).

There are several stages of our solver that can be summarized as follows:

1. Interpret the anonymous handles for the PDO and linear constraints using
   automatic differentiation (see Section 4).

2. Construct a separable representation (a sum of tensor products of linear or-
   dinary differential operators) for the PDO, represent the ordinary differential
   operators with the ultraspherical spectral method (see Section 3), and then
   discretize to form a generalized Sylvester matrix equation with an \(n_y \times n_x\)
   solution matrix (see Section 5).

3. Impose the linear constraints on the solution matrix and solve the resulting
   matrix equation using either a fast Sylvester solver for PDOs of splitting
   rank 2 or a block-banded matrix solver for operators with a splitting rank \(\geq 3\)
   (see Section 6).

4. Apply a resolution check. If the solution is unresolved in the 1st or 2nd
   variable, then increase \(n_x\) or \(n_y\) accordingly, and go back to step 2; otherwise,
   go to step 5.

5. Represent the solution as a chebfun2.

Figure 1.1 summarizes these five stages. Each stage is explained in more detail
in subsequent sections. Throughout the paper we describe the spectral method for
PDEs on \([-1,1] \times [-1,1]\) (to avoid the affine transformations in (1.2)), unless stated
otherwise. The algorithm and software permits linear PDEs defined on bounded
rectangular domains.

In the next section we briefly describe some existing spectral methods for solving
linear PDEs, and in Section 3 we introduce the ultraspherical spectral method. In
Section 4 we define the splitting rank of a PDO and explain how it can be calculated
from the anonymous handle for the operator using automatic differentiation. In Sec-
In Section 5 we show how PDEs can be reduced to a generalized Sylvester matrix equation with linear constraints, and in Section 6 we describe how to solve these constrained matrix equations. Finally, in Section 7 we present several numerical examples showing the generality of the solver before discussing possibilities for future work in Section 8.

Remark An experimental and rapidly developing implementation of the solver is available in the APPROXFUN package [31] written in the Julia language [5], which is significantly faster than the MATLAB implementation. However, it does not currently support all the features described in this paper — e.g., PDOs with a splitting rank of $\geq 3$, automatic differentiation, and certain splitting rank calculations — so we focus on the MATLAB timings throughout, with footnotes of Julia timings for comparison.

2. Existing spectral methods for PDEs. Here, we give a brief survey of the ideas in spectral collocation methods [16, 46], spectral Galerkin methods [39, 23], spectral element methods [35], and hierarchical methods [25]. A more comprehensive survey can be found in [22, 24].

2.1. Spectral collocation methods. Spectral collocation methods or pseudospectral methods are arguably the most convenient and widely applicable spectral method for PDEs. They are usually based on tensor product grids, where the PDO is discretized by its action on values of an interpolating polynomial [16, 46]. In 1D it is well-known that collocation methods lead to dense and typically ill-conditioned linear systems [9]. In 2D the situation is worse as the dense linear systems are typically squared times larger in size and condition number, resulting in $O((n_xn_y)^3)$ complexity. Therefore, 2D collocation methods are restricted to quite small discretization sizes [16, 46].

Typically, collocation methods incorporate linear constraints on the solution by boundary bordering, which replaces rows of a linear system by “boundary” rows [7] that constrain the solution’s values. Sometimes it is not clear which row of the linear system should be replaced and an idea called rectangular spectral collocation can be used to impose boundary rows in a natural way [13]. Boundary bordering requires the construction of a large dense matrix. In Section 4 we show how a separable representation of a partial differential operator with a splitting rank of 2 can be automatically computed and the associated PDE then solved by a fast Sylvester solver. This could be used in conjunction with a collocation method to solve some PDEs without constructing large ill-conditioned linear systems. Unfortunately, there is no convenient way to carry out boundary bordering in the matrix equation setting. Instead, we impose the constraints on the solution by a different, but equally general strategy (see Section 6).
2.2. Spectral Galerkin methods. Spectral Galerkin methods employ global basis functions that usually depend on either the PDE, the linear constraints, or both. They can be derived to respect a particular underlying structure, for instance, self-adjoint elliptic PDEs can be discretized by symmetric linear systems [37, 38]. The resulting matrices can also be well-conditioned and block banded. For example, Shen considers several Chebyshev-based methods for elliptic PDEs [39, 40, 41] and Julian and Watson employs a recombined Chebyshev basis to achieve block banded and well-conditioned linear systems [23].

Galerkin methods usually incorporate any linear constraints by basis recombination, where the basis is constructed so that any linear combination is guaranteed to satisfy the constraints [7]. We find this makes Galerkin methods less applicable for a general PDE solver because designing the “right” basis is often more of an art than a science. For more exotic linear constraints there may not be a convenient basis readily available.

2.3. Operational tau method. The operational tau method requires a tensor product orthogonal polynomial basis, where the PDO is discretized by its action on a matrix of coefficients of a bivariate polynomial [32]. In 2D the resulting linear systems are usually block banded from below but are otherwise dense and ill-conditioned. This approach suffers in a similar way to collocation methods for large discretization sizes.

The operational tau method was popularized and extended by Ortiz and his colleagues [20, 33]. It is a useful scheme for constructing a general PDE solver, but we use the ultraspherical spectral method [30] instead, because it results in well-conditioned matrices and a PDE solver with a lower complexity.

2.4. Spectral element and hierarchical methods. Spectral element methods were introduced in [35] with the underlying principle of combining the generality of finite element methods for complex geometries with the accuracy of spectral methods. Typically, in 2D a domain is partitioned into rectangular regions so that on each subdomain the solution to a PDE can be represented with a low degree bivariate polynomial. Then, each subdomain is solved by a spectral method together with coupling conditions that impose global continuity on the solution. When spectral element methods are employed together with a domain decomposition method [47], such as the Schwarz algorithm [10] or the hierarchical Poincare–Steklov scheme [19], the resulting PDE solver has a complexity of $O(N^{3/2})$ or even $O(N)$, where $N$ is the total number of degrees of freedom used to represent the solution. Such methods always compute solutions that are piecewise smooth, which can lead to a suboptimal number of degrees of freedom required. This is particularly the case for highly oscillatory solutions such as those satisfying the Helmholtz equation with a high wavenumber. The spectral method we describe constructs a globally smooth approximant and hence oscillatory solutions are represented by a near-optimal number of degrees of freedom.

3. The ultraspherical spectral method. A fundamental component of our PDE solver is a spectral method for linear ordinary differential equations (ODEs) that leads to spectrally accurate discretizations and almost banded\footnote{A matrix is almost banded if it is banded except for a small number of columns or rows.} well-conditioned matrices. This section reviews the ultraspherical spectral method (for further details see [30]). This will form the basis of our 2D spectral method.

First, consider a linear ODE with constant coefficients defined on $[-1, 1]$ of the
following form:

\[ a_N \frac{d^N u}{dx^N} + \cdots + a_1 \frac{du}{dx} + a_0 u = f, \quad N \geq 1, \quad (3.1) \]

where \( a_0, \ldots, a_N \) are complex numbers, \( f \) is a univariate function, and \( u \) is the unknown solution. Furthermore, assume that the ODE is supplied with \( K \) linear constraints, i.e., \( \mathcal{B} u = c \) where \( \mathcal{B} \) is a linear operator and \( c \in \mathbb{C}^K \), so that the solution to (3.1) is unique. The ultraspherical spectral method aims to find the solution of (3.1) represented in the Chebyshev basis and compute a vector of Chebyshev expansion coefficients of the solution. That is, the spectral method seeks to find an infinite vector \( \mathbf{u} = (u_0, u_1, \ldots)^T \) such that

\[ u(x) = \sum_{j=0}^{\infty} u_j T_j(x), \quad x \in [-1, 1], \]

where \( T_j \) is the degree \( j \) Chebyshev polynomial.

Classically, spectral methods represent differential operators by dense matrices [7, 16, 46], but the ultraspherical spectral method employs a “sparse” recurrence relation

\[
\frac{d^\lambda T_n}{dx^\lambda} = \begin{cases} 
2^{\lambda-1}n(\lambda - 1)!C_{n-\lambda}^{(\lambda)}, & n \geq \lambda, \\
0, & 0 \leq n \leq \lambda - 1,
\end{cases}
\]

where \( C_j^{(\lambda)} \) is the ultraspherical polynomial with an integer parameter \( \lambda \geq 1 \) of degree \( j \) [29, Sect. 18.3]. This results in a sparse representation of first and higher order differential operators. The differentiation operator for the \( \lambda \)th derivative is given by

\[ \mathcal{D}_\lambda = 2^{\lambda-1}(\lambda - 1)! \begin{pmatrix} \lambda & \lambda+1 & \lambda+2 & \ddots \\ 0 & \lambda & \lambda+1 & \ddots \\ \frac{1}{2} & 0 & \lambda & \ddots \\ \vdots & \ddots & \ddots & \ddots \end{pmatrix}, \quad \lambda \geq 1. \]

For \( \lambda \geq 1 \), \( \mathcal{D}_\lambda \) maps a vector of Chebyshev expansion coefficients to a vector of \( C^{(\lambda)} \) expansion coefficients of the \( \lambda \)th derivative. For \( \lambda = 0 \), \( \mathcal{D}_0 \) is the identity operator.

Since \( \mathcal{D}_\lambda \) for \( \lambda \geq 1 \) returns a vector of ultrasphepherical expansion coefficients, the ultraspherical spectral method also requires conversion operators, denoted by \( \mathcal{S}_\lambda \) for \( \lambda \geq 0 \). The operator \( \mathcal{S}_0 \) converts a vector of Chebyshev coefficients to a vector of \( C^{(1)} \) coefficients and, more generally, \( \mathcal{S}_\lambda \) for \( \lambda \geq 1 \) converts a vector of \( C^{(\lambda)} \) coefficients to a vector of \( C^{(\lambda+1)} \) coefficients. Using the relations in [29, (18.9.7) and (18.9.9)] it can be shown that (see [30] for a derivation)

\[
\mathcal{S}_0 = \begin{pmatrix} 1 & 0 & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \ddots \\
0 & -\frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{2} & \ddots \\
\frac{1}{2} & 0 & -\frac{1}{2} & 0 & \frac{1}{2} & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}, \quad \mathcal{S}_\lambda = \begin{pmatrix} 1 & 0 & -\frac{\lambda}{\lambda+2} & \frac{\lambda}{\lambda+1} & 0 & \frac{\lambda}{\lambda+3} & \ddots \\
0 & -\frac{\lambda}{\lambda+2} & 0 & \frac{\lambda}{\lambda+1} & 0 & \frac{\lambda}{\lambda+3} & \ddots \\
\frac{\lambda}{\lambda+1} & 0 & \frac{\lambda}{\lambda+2} & 0 & \frac{\lambda}{\lambda+3} & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}, \quad \lambda \geq 1.
\]
Note that for $\lambda \geq 1$, the operator $S_0^{-1} \cdots S_{\lambda-1}^{-1}D_\lambda$ is dense and upper-triangular. This is the operator that represents $\lambda$th order differentiation in the Chebyshev basis without converting to ultraspherical bases [32]. It is upper-triangular but otherwise dense.

We can combine our conversion and differentiation operators to represent the ODE in (3.1) as follows:

$$(a_N D_N + a_{N-1} S_{N-1} D_{N-1} + \cdots + a_0 S_0 \cdots S_0 D_0) u = S_{N-1} \cdots S_0 f,$$  

(3.2)

where $u$ and $f$ are vectors of Chebyshev expansion coefficients of $u$ and $f$, respectively. The conversion operators are used in (3.2) to ensure that the resulting linear combination maps Chebyshev coefficients to $C^N$ coefficients, and the right-hand side $f$ is represented by a vector of $C^N$ expansion coefficients.

To make the solution to (3.2) unique we must impose the $K$ prescribed linear constraints in $B$ on $u$. That is, we must represent the action of the linear constraints on a vector of Chebyshev coefficients. For example, Dirichlet boundary conditions take the form

$$B = \begin{pmatrix} T_0(-1) & T_1(-1) & T_2(-1) & T_3(-1) & \cdots \\ T_0(1) & T_1(1) & T_2(1) & T_3(1) & \cdots \end{pmatrix} = \begin{pmatrix} 1 & -1 & 1 & -1 & \cdots \\ 1 & 1 & 1 & 1 & \cdots \end{pmatrix},$$

because $Bu = (u(-1), u(1))^T$, and Neumann conditions at $x = \pm 1$ take the form

$$B = \begin{pmatrix} T_0'(-1) & T_1'(-1) & T_2'(-1) & T_3'(-1) & \cdots \\ T_0'(1) & T_1'(1) & T_2'(1) & T_3'(1) & \cdots \end{pmatrix} = \begin{pmatrix} 0 & -1 & 4 & -9 & \cdots \\ 0 & 1 & 4 & 9 & \cdots \end{pmatrix},$$

because $Bu = (u'(-1), u'(1))^T$. In general, any linear constraint can be represented by its action on a vector of Chebyshev coefficients.

Finally, to construct a linear system that can be solved for the first $n$ Chebyshev coefficients of $u$ we take the $n \times n$ finite section. Let $P_n$ be the truncation operator that maps $C^\infty$ to $C^n$ such that $P_n u = (u_0, \ldots, u_{n-1})^T$. We take the first $n$ columns of $B$, $B = BP_n^T$, the $(n-K) \times n$ principal submatrix of $L$, $L = P_{n-K} L P_n^T$, and form the following linear system:

$$\begin{pmatrix} B \\ L \end{pmatrix} P_n u = \begin{pmatrix} c \\ P_{n-K} S_{n-1} \cdots S_0 f \end{pmatrix}.$$  

(3.3)

Since the operators $D_\lambda$ and $S_\lambda$ are banded, the matrix $L$ is banded, and the resulting linear system is almost banded, i.e., banded except for $K$ rows imposing the linear constraints on $u$. The $K$ rows in (3.3) that impose the linear constraints could also be placed below $L$, but we place them above so that the linear system has a structure that is as close as possible to upper-triangular.

### 3.1. Multiplication matrices.

For ODEs with variable coefficients we need to be able to represent the multiplication operation $M[a]u = a(x)u(x)$. Since the ultraspherical spectral method converts between different ultraspherical bases, we need to construct multiplication matrices for each ultraspherical basis.

Suppose we wish to represent $M[a]u$, where $a(x)$ and $u(x)$ have Chebyshev expansions

$$a(x) = \sum_{j=0}^\infty a_j T_j(x), \quad u(x) = \sum_{j=0}^\infty u_j T_j(x),$$
Fig. 3.1. Left: Typical structure of the matrices constructed by the ultraspherical spectral method, i.e., banded matrices except for a small number of dense rows. Right: The solution of $\epsilon u''(x) + xu'(x) + \sin(x)u(x) = 0$, $u(\pm1) = 1$, for $\epsilon = 10^{-1}, 10^{-3}, 10^{-7}$. The ultraspherical spectral method typically constructs well-conditioned matrices and hence, can resolve solutions that require large linear systems.

and we desire the Chebyshev expansion coefficients of $a(x)u(x)$. Define $M_0[a]$ to be the operator that takes the vector of Chebyshev expansion coefficients of $u(x)$ and returns the vector of Chebyshev expansion coefficients of $a(x)u(x)$. It is shown in [30] that $M_0[a]$ can be written as the following Toeplitz-plus-Hankel-plus-rank-1 operator:

$$M_0[a] = \frac{1}{2} \begin{bmatrix} 2a_0 & a_1 & a_2 & a_3 & \cdots \\ a_1 & 2a_0 & a_1 & a_2 & \cdots \\ a_2 & a_1 & 2a_0 & a_1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots \\ a_1 & a_2 & a_3 & a_4 & \cdots \\ a_2 & a_3 & a_4 & a_5 & \cdots \\ a_3 & a_4 & a_5 & a_6 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

This multiplication operator looks dense; however, if $a(x)$ is approximated by a polynomial of degree $m$, then $M_0[a]$ is banded with a bandwidth of $m$.

We also require multiplication operators $M_\lambda[a]$ that represent multiplication of two $C^{(\lambda)}$ series. That is, if $u$ is a vector of Chebyshev expansion coefficients of $u$, then the sequence of matrices $M_\lambda[a]S_{\lambda-1} \cdots S_0u$ returns the $C^{(\lambda)}$ expansion coefficients of $a(x)u(x)$. In [30] an explicit formula for the entries of $M_\lambda[a]$ for $\lambda \geq 1$ is given and in [45, Chap. 6] it is shown that $M_\lambda[a]$ satisfy a three-term recurrence relation.

Figure 3.1 (left) shows the typical structure of the nonzero entries in a linear system. The linear system in (3.3) can be solved in $O(n)$ operations by the QR factorization applied to a “filled-in” representation [30]. Furthermore, an adaptive procedure based on (F. W. J.) Olver’s algorithm [28] can be derived to find the minimum value of $n$ required to resolve the solution to machine precision with essentially no extra cost.

Remarkably, this spectral method constructs not only almost banded matrices, but typically well-conditioned ones too [30, Lemma 4.4]. Therefore, the ultraspherical spectral method is not plagued with the ill-conditioning associated to classical spectral methods. Figure 3.1 (right) shows the solution to a singularly perturbed boundary value problem, $\epsilon u''(x) + xu'(x) + \sin(x)u(x) = 0$, $u(\pm1) = 1$, for $\epsilon = 10^{-1}, 10^{-3}, 10^{-7}$. For $\epsilon = 10^{-7}$ a Chebyshev expansion of degree 22,950 is required to approximate
the solution to machine precision. We also observe high accuracy of the 2D spectral method we derive in this paper (see Section 7).

4. Automatic differentiation and separable representations. We now describe the implementation and mathematics behind our 2D linear PDE solver. The user interface accepts input of a PDO as an anonymous handle, in a syntax that closely resembles how the equation is written in standard textbooks. This is achieved in two main steps: (1) Interpret the anonymous handle for the PDO using automatic differentiation (see Section 4.1), and (2) Calculate a separable representation for the PDO (see Sections 4.2 and 4.3). Once a separable representation has been constructed the PDE can be discretized by using the 1D ultraspherical spectral method.

4.1. Interpreting user-defined input using automatic differentiation. The Chebop2 interface uses automatic differentiation, more precisely, forward-mode operator overloading, which allows it to extract out the variable coefficients of a PDO given only an anonymous handle for the operator. A description of how to overload operators in MATLAB and implement automatic differentiation is given in [27].

As an example, suppose a user wants to solve a PDE with the differential equation

\[ u_{xx} + u_{yy} + K^2 u + yu = f. \]

The user could type the following into Chebop2:

\[ N = \text{chebop2}(@(x,y,u) \text{diff}(u,2,2) + \text{diff}(u,2,1) + k^2 u + y.*u); \]

From this anonymous handle the solver derives all it needs to know about how to discretize the operator.

First, we evaluate the anonymous handle at objects \( x, y, \) and \( u \) from MATLAB classes that have their own versions of \( \text{diff}, +, \cdot, \) and \( .\cdot \) (the elementary operations in the anonymous handle). Then, as the handle is evaluated, these elementary operations are executed in a particular sequence, with each one not only computing the expected quantity but also updating an array for the variable coefficients. Since the individual operations are elementary, there is a simple rule on how each one should update the array of variable coefficients. Once complete, we have as a byproduct of the evaluation of the anonymous handle, an array containing the variable coefficients of the PDO. The MATLAB classes for \( x, y, \) and \( u \) have a growing dictionary of overloaded elementary operations so the user can express a PDO in a multitude of ways. A similar process is used to extract information from user input for the linear constraints for the PDE.

Figure 4.1 shows how \( u_{xx} + u_{yy} + K^2 u + yu \) can be constructed by combining elementary operations. As the anonymous handle is evaluated, the tree is traversed from the leaves to the root node and at each node the variable coefficients of the PDO are updated.

4.2. Separable representations of partial differential operators. A separable representation of a 2D object is a sum of “products” of 1D objects and in the case of linear PDOs those 1D objects are linear ordinary differential operators (ODOs). An ODO is the operator associated to an ODE, such as (3.1), and acts on sufficiently smooth univariate functions. It can be written as a finite linear combination of differential and multiplication operators.

A nonzero linear PDO has a splitting rank of 1 if it can be expressed as an tensor product of two ODOs, written as \( (\mathcal{O}_y \otimes \mathcal{O}_x) \), which acts on sufficiently smooth bivariate functions. A linear PDO, \( \mathcal{L} \), has a splitting rank of \( \leq k \) if it can be written as a sum of \( k \) tensor products of ODOs,

\[ \mathcal{L} = \sum_{j=1}^{k} (\mathcal{O}_y^j \otimes \mathcal{O}_x^j), \]
Fig. 4.1. A tree that shows how the expression \( u_{xx} + u_{yy} + K^2u + yu \) can be constructed from \( x, y, u, \) and elementary operations. A tree can be traversed in an object-oriented language such as Matlab by a simple automatic differentiation technique known as forward-mode operator overloading and in the process the variable coefficients for \( u_{xx} + u_{yy} + K^2u + yu \) can be determined.

and the splitting rank\(^2\) of a PDO is the minimum number of terms in such a representation.

**Definition 4.1.** Let \( \mathcal{L} \) be a linear PDO in the form (1.1). The splitting rank of \( \mathcal{L} \) is the smallest integer \( k \) for which there exist linear ODOs \( \mathcal{L}^{y1}, \ldots, \mathcal{L}^{yk} \) (acting on functions in \( y \)) and \( \mathcal{L}^{x1}, \ldots, \mathcal{L}^{xk} \) (acting on functions in \( x \)) that satisfy

\[
\mathcal{L} = \sum_{j=1}^{k} (\mathcal{L}^{yj} \otimes \mathcal{L}^{xj}).
\] (4.1)

A linear PDO of finite differential order with polynomial variable coefficients must itself have a finite splitting rank. To have an infinite splitting rank, one of its variable coefficients must be of infinite mathematical rank (for a definition of the rank of a smooth bivariate function, see [45]).

4.3. **Determining the splitting rank of a partial differential operator.**

One way to determine the splitting rank of a PDO is directly from Definition 4.1. For example, the splitting rank of the Helmholtz operator \( \partial^2/\partial x^2 + \partial^2/\partial y^2 + K^2 \) is 2 since

\[
\partial^2/\partial x^2 + \partial^2/\partial y^2 + K^2 = (\mathcal{I} \otimes \mathcal{D}^2) + ((\mathcal{D}^2 + K^2) \otimes \mathcal{I}),
\]

where \( \mathcal{I} \) is the identity operator and \( \mathcal{D} \) is the first order differential operator. Furthermore, it can be shown that the splitting rank of \( \partial^2/\partial x^2 + \partial^2/(\partial x \partial y) + \partial^2/\partial y^2 \) is 3 and the splitting rank of \( (2 + \sin(x + y))\partial^2/\partial x^2 + e^{-(x^2+y^2)}\partial^2/\partial y^2 \) is 4. Another way, which allows it to be calculated by a computer, uses a technique motivated by umbral calculus [4].

**Proposition 4.2.** Let \( \mathcal{L} \) be a linear PDO in the form (1.1) with variable coefficients of finite rank. The splitting rank of \( \mathcal{L} \) is equal to the smallest integer \( k \) required

---

\(^2\)Our definition of splitting rank differs from the rank of a linear operator in functional analysis. All nontrivial PDOs are of infinite rank, but usually have a finite splitting rank.
in an expression of the form

\[
\sum_{i=0}^{N_y} \sum_{j=0}^{N_x} \ell_{ij}(s,t) y^i x^j = \sum_{j=1}^{k} c_j(t,y) r_j(s,x),
\]

(4.2)

where \(c_j\) and \(r_j\) are bivariate functions.

Proof. Let \(T\) be the linear operator defined by

\[
T [\ell(s,t)y^i x^j] = \ell(x,y) \frac{\partial^{i+j}}{\partial y^i \partial x^j}, \quad i, j \geq 0,
\]

which replaces \(s\) and \(t\) by \(x\) and \(y\) and powers of \(x\) and \(y\) by partial derivatives. Now, suppose that \(L\) is a linear PDO with a splitting rank of \(r\) and \(k\) is the minimum number of terms required in (4.2). We will show that \(r = k\).

First, note that the linear operator \(T\) can be used to give the following relation:

\[
L = \sum_{i=0}^{N_y} \sum_{j=0}^{N_x} \ell_{ij}(s,t) y^i x^j = T \left[ \sum_{i=0}^{N_y} \sum_{j=0}^{N_x} \ell_{ij}(s,t) y^i x^j \right] = T [H(s,x,t,y)],
\]

where \(H(s,x,t,y) = \sum_{i=0}^{N_y} \sum_{j=0}^{N_x} \ell_{ij}(s,t) y^i x^j\). Now, if the function \(H(s,x,t,y)\) can be written as \(\sum_{j=1}^{k} c_j(t,y) r_j(s,x)\), then we have

\[
L = \sum_{j=1}^{k} c_j(t,y) r_j(s,x) = \sum_{j=1}^{k} T [c_j(t,y) r_j(s,x)] = \sum_{j=1}^{k} T [c_j(t,y)] \otimes T [r_j(s,x)],
\]

where \(T[c_j(t,y)]\) and \(T[r_j(s,x)]\) are ODOs with variable coefficients in \(y\) and \(x\), respectively, and hence \(r \leq k\). Conversely, a separable representation for \(L\) can be converted (using \(T\)) to a low rank expression for \(H\), and hence \(k \leq r\). We conclude that \(r = k\) and the splitting rank of \(L\) equals the minimum number of terms required in (4.2). □

A special case of Proposition 4.2 gives a connection between constant coefficient PDOs and bivariate polynomials. This connection has been previously used to investigate polynomial systems of equations [42, Chap. 10]. In particular, if \(L\) has constant coefficients, then the splitting rank of \(L\) can be calculated as the rank of a bivariate polynomial using the singular value decomposition of a function [44]. In general, for linear PDOs with variable coefficients the splitting rank of \(L\) is the splitting rank of a function of four variables and can be calculated using a tensor-train decomposition of a function [34].

More generally, Proposition 4.2 allows us to calculate a separable representation for a linear PDO via a low rank representation of the associated function in (4.2). Each term in the separable representation involves a tensor product of two linear ODOs, which can be discretized using the 1D ultraspherical spectral method (see Section 3). In Section 6 a PDO with a splitting rank of \(k\) will be discretized by a generalized Sylvester equation with \(k\) terms.

Quite surprisingly many standard linear PDOs have a splitting rank of 2 and Table 4.1 presents a selection. Usually, but not always, a linear PDO with variable coefficients has a splitting rank of \(\geq 3\) and any ODO is a PDO with a splitting rank of 1.

3The definition of this operator is motivated by umbral calculus [4].
PDO Operator

<table>
<thead>
<tr>
<th>PDO</th>
<th>Operator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laplace</td>
<td>$u_{xx} + u_{yy}$</td>
</tr>
<tr>
<td>Helmholtz</td>
<td>$u_{xx} + u_{yy} + K^2u$</td>
</tr>
<tr>
<td>Heat</td>
<td>$u_t - \alpha^2 u_{xx}$</td>
</tr>
<tr>
<td>Transport</td>
<td>$u_t - bu_{xx}$</td>
</tr>
<tr>
<td>Wave</td>
<td>$u_{tt} - c^2 u_{xx}$</td>
</tr>
<tr>
<td>Euler–Tricomi</td>
<td>$u_{xx} - xu_{yy}$</td>
</tr>
<tr>
<td>Schrödinger</td>
<td>$i\epsilon u_t + \frac{1}{2}\epsilon^2 u_{xx} - V(x)u$</td>
</tr>
<tr>
<td>Black–Scholes</td>
<td>$u_t + \frac{1}{2}\sigma^2 x^2 u_{xx} + rxu_x - ru$</td>
</tr>
</tbody>
</table>

Table 4.1

A selection of PDOs with a splitting rank of 2 (see Definition 4.1). Many constant coefficient PDOs have a splitting rank of 2. An exception is the biharmonic operator, which has a splitting rank of 3.

5. Discretization of a separable representation for a partial differential operator. Any PDO with a splitting rank of $k$ (see (4.1)) can be discretized to a generalized Sylvester matrix equation with $k$ terms, $A_1XC_1^T + \cdots + A_kXC_k^T$, where the matrices $A_1, \ldots, A_k$ and $C_1, \ldots, C_k$ are ultraspherical spectral discretizations of ODOs and $X$ is a matrix containing the bivariate Chebyshev expansion coefficients of the solution.

Specifically, suppose we seek to compute a matrix $X \in \mathbb{C}^{n_y \times n_x}$ of bivariate Chebyshev expansion coefficients of the solution $u(x,y)$ to (1.1) satisfying

$$\left| u(x,y) - \sum_{i=0}^{n_y} \sum_{j=0}^{n_x} X_{ij} T_i(y) T_j(x) \right| \leq \mathcal{O}(\epsilon \|u\|_{\infty}), \quad (x,y) \in [-1,1]^2,$$

(5.1)

where $\epsilon$ is machine precision. The ultraspherical spectral method can be used to represent the ODOs $\mathcal{L}_{y}^1, \ldots, \mathcal{L}_{y}^k$ and $\mathcal{L}_{x}^1, \ldots, \mathcal{L}_{x}^k$ in (4.1) as matrices $\mathcal{L}_{y}^1, \ldots, \mathcal{L}_{y}^k$ and $\mathcal{L}_{x}^1, \ldots, \mathcal{L}_{x}^k$. These matrices can be truncated to derive the following generalized Sylvester matrix equation:

$$A_1XC_1^T + \cdots + A_kXC_k^T = F,$$

(5.2)

where $A_j = \mathcal{P}_{n_y} \mathcal{L}_{y}^j \mathcal{P}_{n_x}$ and $C_j = \mathcal{P}_{n_x} \mathcal{L}_{x}^j \mathcal{P}_{n_y}$ for $1 \leq j \leq k$, and $F$ is the $n_y \times n_x$ matrix of bivariate Chebyshev expansion coefficients for the right-hand side $f$ in (1.1).

Typically, the matrix equation (5.2) does not have a unique solution as the prescribed linear constraints $\mathcal{B}_x$ and $\mathcal{B}_y$ must also be incorporated. By investigating the action of $\mathcal{B}_x$ on the basis $\{T_0(x), \ldots, T_{n_x-1}(x)\}$, we can discretize any linear constraint of the form $\mathcal{B}_x u(x,y) = g(y)$ as $XB_x^T = G^T$, where $B_x$ is an $K_x \times n_x$ matrix and $G$ is an $K_x \times n_y$ matrix containing the first $n_y$ Chebyshev coefficients of each component of $g$. Similarly, by investigating the action of $\mathcal{B}_y$ on the basis $\{T_0(y), \ldots, T_{n_y-1}(y)\}$ we can discretize $\mathcal{B}_y u(x,y) = h(x)$ as $B_y X = H$.  

12
where $H$ is an $K_y \times n_x$ matrix containing the first $n_x$ Chebyshev coefficients of each component of $h$.

For the constraints to be consistent the matrices $B_x$ and $B_y$ must satisfy the following compatibility conditions:

$$HB_x^T = (B_yX)B_x^T = B_y(XB_x^T) = B_yG^T. \quad (5.3)$$

For example, in order that Dirichlet conditions satisfy the compatibility conditions the boundary data must match at the four corners of $[-1,1]^2$. Section 6 describes how to solve matrix equations of the form (5.2) with linear constraints.

In practice, the solver determines the parameters $n_x$ and $n_y$ by progressively discretizing the PDE on finer and finer grids until the solution is resolved. First, we discretize the PDE with $n_x = n_y = 9$ and solve the resulting matrix equation (5.2) under linear constraints (see Section 6). Then, we check if the Chebyshev coefficients in $X$ decay to below machine precision relative to the maximum entry of $X$ in absolute value. Roughly speaking, if the last few columns of $X$ are above relative machine precision, then the solution has not been resolved in the $x$-variable and $n_x$ is increased to 17, 33, 65, and so on, and likewise if the last few rows in $X$ are above relative machine precision, then $n_y$ is increased to 17, 33, 65, and so on. The exact resolution tests we employ are the same as those employed by Chebfun2 [43], which are heuristic in nature, but based on a significant amount of practical experience. The discretization parameters $n_x$ and $n_y$ are independently increased and the resolution test is performed in both directions after each solve. Usually, this means that the final solution satisfies (5.1), though it is not an absolute guarantee.


In this section we describe how to solve the following matrix equation with linear constraints:

$$\sum_{j=1}^{k} A_j XC_j^T = F, \quad X \in \mathbb{C}^{n_y \times n_x}, \quad B_yX = H, \quad XB_x^T = G^T, \quad (6.1)$$

where $A_j \in \mathbb{C}^{n_y \times n_x}$, $C_j \in \mathbb{C}^{n_x \times n_x}$, $F \in \mathbb{C}^{n_y \times n_x}$, $B_y \in \mathbb{C}^{K_y \times n_y}$, $B_x \in \mathbb{C}^{K_x \times n_x}$, $H \in \mathbb{C}^{K_x \times n_x}$, and $G \in \mathbb{C}^{K_y \times n_y}$. Our approach is to use the linear constraints to remove degrees of freedom in $X$ and thus obtain a generalized Sylvester matrix equation with a unique solution without constraints.

By assumption the prescribed linear constraints are linearly independent so the column ranks of $B_x$ and $B_y$ are $K_x$ and $K_y$, respectively. Without loss of generality, we further assume that the principal $K_x \times K_x$ and $K_y \times K_y$ submatrices of $B_x$ and $B_y$ are the identity matrices$^4$ $I_{K_x}$ and $I_{K_y}$. Then, we can modify the matrix equation in (6.1) to

$$\sum_{j=1}^{k} A_j XC_j^T - \sum_{j=1}^{k} (A_j)_{1:n_y,1:K_y} B_y XC_j^T = F - \sum_{j=1}^{k} (A_j)_{1:n_y,1:K_y} HC_j^T,$$

where we have used the constraint $B_yX = H$. Moreover, by rearranging we have

$$\sum_{j=1}^{k} A_j XC_j^T - \sum_{j=1}^{k} (A_j)_{1:n_y,1:K_y} B_y XC_j^T = \sum_{j=1}^{k} (A_j - (A_j)_{1:n_y,1:K_y} B_y) XC_j^T,$$

$^4$Otherwise, permute the columns of $B_x$ and $B_y$, and the corresponding rows/columns of $X$, so the principal $K_x \times K_x$ and $K_y \times K_y$ matrices $\hat{B}_x$ and $\hat{B}_y$ are invertible, then redefine as $B_x \mapsto \hat{B}_x^{-1}B_x$, $G \mapsto \hat{B}_x^{-1}G$, $B_y \mapsto \hat{B}_y^{-1}B_y$, and $H \mapsto \hat{B}_y^{-1}H$. 13
and since the \( K_y \times K_y \) principal matrix of \( B_y \) is the identity matrix, each matrix \( A_j - (A_j)_{1:n_x,1:K_y}B_y \) for \( 1 \leq j \leq k \) is zero in the first \( K_y \) columns. Similarly, the condition \( XB_x^T = G^T \) can be used to further modify the matrix equation as follows:

\[
\sum_{j=1}^{k} (A_j - (A_j)_{1:n_x,1:K_y}B_y) X (C_j - B_x(C_j)_{1:n_x,1:K_y})^T = F - \sum_{j=1}^{k} (A_j - (A_j)_{1:n_x,1:K_y}B_y) HC_j^T - \sum_{j=1}^{k} (A_j - (A_j)_{1:n_x,1:K_y}B_y) G^T (C_j)_{1:n_x,1:K_y}^T,
\]

so that the matrices \((C_j - B_x(C_j)_{1:n_x,1:K_y})^T\) for \( 1 \leq j \leq k \) are zero in the first \( K_x \) rows.

Now, the first \( K_y \) columns of \( A_j - (A_j)_{1:n_x,1:K_y}B_y \) and the first \( K_x \) rows of \((C_j - B_x(C_j)_{1:n_x,1:K_y})^T\) are zero in (6.2) and hence, the matrix equation is independent of the first \( K_y \) rows and \( K_x \) columns of \( X \). Therefore, the matrix equation in (6.2) can be reduced by removing those columns and rows and then solved, obtaining a matrix \( X_{22} \in \mathbb{C}^{(n_y - K_y) \times (n_x - K_x)} \), where

\[
X = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix}, \quad X_{11} \in \mathbb{C}^{K_y \times K_x}, \quad X_{12} \in \mathbb{C}^{K_y \times (n_x - K_x)}, \quad X_{21} \in \mathbb{C}^{(n_y - K_y) \times K_x}.
\]

The solution of the resulting unconstrained generalized Sylvester equation that \( X_{22} \) satisfies is given in Section 6.1.

Once we have computed \( X_{22} \) we can recover \( X \) by using the linear constraints. For instance, since \( B_yX = H \) and the \( K_y \times K_y \) principal submatrix of \( B_y \) is the identity matrix, we have

\[
X_{12} = H_2 - B^{(2)}_y X_{22},
\]

where \( H = [H_1, H_2] \) with \( H_1 \in \mathbb{C}^{K_y \times K_x} \) and \( H_2 \in \mathbb{C}^{K_y \times (n_x - K_x)} \), and \( B_y = [I_{K_y}, B^{(2)}_y] \) with \( B^{(2)}_y \in \mathbb{C}^{K_y \times (n_y - K_y)} \). Furthermore, since \( XB_x^T = G^T \) and the \( K_x \times K_x \) principal submatrix of \( B_x \) is the identity matrix, we have

\[
X_{21} = G_2^T - X_{22}(B^{(2)}_x)^T,
\]

where \( G = [G_1, G_2] \) with \( G_1 \in \mathbb{C}^{K_x \times K_x} \) and \( G_2 \in \mathbb{C}^{K_x \times (n_x - K_x)} \), and \( B_x = [I_{K_x}, B^{(2)}_x] \) with \( B^{(2)}_x \in \mathbb{C}^{K_x \times (n_x - K_x)} \). Lastly, we can recover \( X_{11} \) using either of the two formulas

\[
X_{11} = H_1 - B^{(2)}_y X_{21}, \quad X_{11} = G_1^T - X_{12}(B^{(2)}_x)^T,
\]

since the compatibility condition (5.3) ensures that both formulas are equivalent.

6.1. Solving a generalized Sylvester matrix equation. We are left with a standard generalized Sylvester matrix equation of the form

\[
\sum_{j=1}^{k} \tilde{A}_j X_{22} \tilde{C}_j^T = \tilde{F},
\]

and the exact algorithm we use to solve for \( X_{22} \) depends on \( k \).

If \( k = 1 \) then the matrix equation takes the form \( A_1 X_{22} C_1^T = \tilde{F} \), and since we are using the ultraspherical spectral method (see Section 3) the matrices \( A_1 \) and \( C_1 \)
are almost banded. Therefore, we can solve $\tilde{A}_1 Y = \tilde{F}$ for $Y \in \mathbb{C}^{(n_y-K_y) \times (n_x-K_x)}$ in $O(n_xn_y)$ operations and then solve $\tilde{C}_1 X_{22}^T = Y^T$ for $X_{22}$ in $O(n_xn_y)$ operations using the adaptive QR method [30].

If $k = 2$ then the matrix equation takes the form

$$\tilde{A}_1 X_{22} \tilde{C}_1^T + \tilde{A}_2 X_{22} \tilde{C}_2^T = \tilde{F},$$

(6.4)

To solve (6.4) we use the generalized Bartels–Stewart algorithm [2, 18], which requires $O(n_x^3 + n_y^3)$ operations. Alternatively, the generalized Hessenberg–Schur algorithm can be used [18]. It turns out that many standard PDOs with constant coefficients have a splitting rank of 2 (see Table 4.1).

For $k \geq 3$, we are not aware of an efficient algorithm for solving (6.3). Instead, we expand the matrix equation into an $(n_x-K_x)(n_y-K_y) \times (n_x-K_x)(n_y-K_y)$ linear system

$$\left( \sum_{j=1}^{k} (\tilde{C}_j \otimes \tilde{A}_j) \right) \text{vec}(X_{22}) = \text{vec}(\tilde{F}),$$

(6.5)

where ‘$\otimes$’ denotes the Kronecker product operator for matrices and $\text{vec}(C)$ denotes the vectorization of the matrix $C$ formed by stacking the columns of $C$ into a single column vector.

Naïvely solving the resulting linear system (6.5) requires $O((n_xn_y)^3)$ operations. However, because we are using the ultraspherical spectral method the matrices $\tilde{A}_j$ and $\tilde{C}_j$ are almost banded and hence, the matrix $\sum_{j=1}^{k} (\tilde{C}_j \otimes \tilde{A}_j)$ is also almost banded with a bandwidth of $O(n_x)$ except for $O(n_x)$ dense rows. Thus, the linear system can be solved in $O(n_x^2(n_xn_y)) = O(n_x^3n_y)$ operations using the adaptive QR method [30]. Alternatively, the roles of $x$ and $y$ can be swapped and the linear system solved in $O(n_x^3n_y)$ operations.

Figure 6.1 shows the computational time for solving $\tilde{A}_1 X_{22} \tilde{C}_1^T = \tilde{F}$, (6.4), and (6.5), where the matrices are almost banded with a bandwidth of 10. The typical dominating computational cost of the solver for PDOs with splitting rank 1, 2, and $k \geq 3$ is the matrix equation solve. In particular, Figure 6.1 shows the substantial
efficiency gain that can be achieved when the splitting rank structure of a PDO is exploited.

6.2. Solving subproblems. If the even and odd modes of the solution decouple, then the computational cost can be reduced by solving for them separately. For example, Laplace’s equation with Dirichlet conditions can be split into four subproblems since the PDO contains only even order derivatives in $x$ and $y$ and the boundary conditions can be equivalently written as

$$B_x = \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & \cdots \\ 0 & 1 & 0 & 1 & 0 & \cdots \end{pmatrix}, \quad B_y = \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & \cdots \\ 0 & 1 & 0 & 1 & 0 & \cdots \end{pmatrix}. $$

This means that the even and odd modes decouple and in this case, since the Laplace operator has a splitting rank of 2, the computational cost is reduced by a factor of 8 by solving four subproblems.

In fact, any PDO with constant coefficients that contains only even (or odd) order derivatives in one variable accompanied with pure Dirichlet or pure Neumann boundary conditions decouples into two subproblems. Moreover, if it contains only even (or odd) order derivatives in both variables then it decouples into four subproblems. Our implementation automatically detects these cases and splits the problem into two or four subproblems as appropriate.

7. Numerical examples. We now demonstrate our 2D spectral method on five examples. A MATLAB implementation is available as part of Chebfun [12] via the chebop2 command. An experimental implementation is also available in the APPROXFUN package [31] written in the Julia language [5], and timings are given for comparison.

Example 1: The Helmholtz equation. First, we consider the Helmholtz equation $u_{xx} + u_{yy} + K^2 u = 0$ on $[-1,1]^2$ with Dirichlet boundary conditions, where $K$ is some wavenumber. This simple example is used to verify that our global spectral method resolves oscillatory solutions with an average of $\pi$ degrees of freedom per wavelength. In particular, we set $K = \sqrt{2}\omega$ and solve

$$u_{xx} + u_{yy} + (\sqrt{2}\omega)^2 u = 0, \quad u(\pm1, y) = u(x, \pm1) = f(x, \pm1), \quad (7.1)$$

where $\omega \in \mathbb{R}$ and $f(x, y) = \cos(\omega x) \cos(\omega y)$. The exact solution is $u = f$. In Figure 7.1 we plot the solution for $\omega = 50$ and plot the Cauchy error for $\omega = 10\pi, 50\pi, 100\pi$. The Cauchy error shows that the solution is rapidly resolved once $\pi$ degrees of freedom per wavelength are used (in agreement with the Shannon–Nyquist sampling rate [36]).

For $\omega = 100\pi$ in (7.1) we have

$$\left( \int_{-1}^{1} \int_{-1}^{1} (\hat{u}(x,y) - u(x,y))^2 \, dx \, dy \right)^{\frac{1}{2}} = 5.44 \times 10^{-10} ,$$

where $u$ is the exact solution and $\hat{u}$ is the computed solution. This error is relatively small considering that the solution has more than 20,000 local extrema in $[-1,1]^2$. The solution $\hat{u}$ was computed in 6.06 seconds. (The Julia implementation takes 3.90 seconds.) The implementation automatically set up subproblems, which reduced the computational time by a factor of about 8.

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5Experiments were performed on a 2012 1.8GHz Intel Core i7 MacBook Air with MATLAB 2012a.
Example 2: A variable coefficient Helmholtz equation. Next, to make the Helmholtz equation more challenging we add a variable wave number and a forcing term. For instance, consider $\nabla^2 u + 10000(1/2 + \sin(x)^2)\cos(y)^2 u = \cos(xy)$ on $[-1, 1]^2$ with Dirichlet data. This can be solved in chebop2 with the following syntax:

\[
N = \text{chebop2}(@(x,y,u) \nabla^2(u) + 10000(0.5 + \sin(x)^2)\cdot\cos(y)^2\cdot u); \n\]

\[
N.lbc = 1; N.rbc = 1; N.ubc = 1; N.dbc = 1; \n\]

\[
u = N \backslash \text{chebfun2}(@(x,y) \cos(x\cdot y)); \n\]

The splitting rank of the corresponding PDO is 2, which can be calculated automatically by using Proposition 4.2 and this structure can then be used to discretize the PDE as a generalized Sylvester matrix equation of the form (6.4). Figure 7.2 shows a surface plot of the solution and a Cauchy error plot. The convergence behavior of the Cauchy error is typical for Helmholtz equations: For low discretization sizes there is no decay of the Cauchy error (more degrees of freedom are required to reach Nyquist’s sampling rate), followed by a short-lived but rapid geometric or super-geometric decay (resolving the smooth part of the solution), and then a slower algebraic decay of the error (resolving the weak corner singularity of the solution). Our 2D spectral method allows for quite large discretization sizes, so despite only algebraic decay the solution can still be resolved to a high accuracy.

Example 3: The wave equation and the Klein–Gordon equation. Next we consider the wave equation $u_{tt} = u_{xx}$ modeling a string of length 2 being plucked with a force $u(x, 0) = e^{-50(x-2/10)^2}$ and $u_t(x, 0) = 0$, held fixed on the left $u(-1, t) = 0$, and held by a vertical elastic band on the right $u(1, t) + 5u_x(1, t) = 0$. The string is left to vibrate freely for 10 units of time. We will compare this solution to that of the Klein–Gordon equation $u_{tt} = u_{xx} - 5u$ with the same boundary conditions. The latter equation can be solved by the following CHEBOP2 code:

\[
N = \text{chebop2}(@(u) \text{diff}(u,2,1) - \text{diff}(u,2,2) + 5\cdot u, \{-1 1 0 10\}); \n\]

\[
N.lbc = 0; N.rbc = @(t,u) u/5 + \text{diff}(u); \n\]

\[
N.dbc = @(x,u) [u - \exp(-50\cdot(x-.2)^2) \cdot \text{diff}(u)]; \n\]

\[
u = N \backslash 0; \n\]

In Figure 7.3 we plot the solutions side-by-side. It can be seen that the solution to the wave equation (left) has the initial pulse traveling at a constant speed reflecting with equal and opposite amplitude off the left and with equal sign (but not quite
equal amplitude) from the right. This is typical reflection behavior of traveling waves with these boundary conditions. In contrast, in the solution to the Klein–Gordon equation (right) high frequencies of the pulse travel faster than low frequencies and interference quickly destroys any regular pattern. We require about 2.02 seconds to resolve the Klein–Gordon solution to 8-digits of accuracy with a (92,257) degree bivariate polynomial. (The Julia implementation takes 0.89 seconds.)

**Example 4: The time-dependent Schrödinger equation.** For the fourth example we consider the time-dependent Schrödinger equation on $[0,1] \times [0,0.54]$,

$$i \epsilon u_t = -\frac{1}{2} \epsilon^2 u_{xx} + V(x)u,$$

with $u(0,t) = 0$, $u(1,t) = 0$, and an initial condition $u(x,0) = u_0(x)$, where

$$u_0(x) = e^{-25(x-1/2)^2} e^{-i/(5\epsilon) \log(2 \cosh(5(x-1/2)))}. \tag{7.2}$$
In Figure 7.4 we take $\epsilon = 0.0256$ and plot the real part of the solution when $V(x) = 10$ (left) and $V(x) = x^2$ (right). In both cases, we see the formation of a caustic.

In Figure 7.5 we plot $|u(x, 0.54)|^2$ where $u$ is the solution to (7.2) with $V(x) = 10$ and $\epsilon = 0.0064$ (left). Our results are consistent with [1, Fig. 2b], which used periodic boundary conditions in place of Dirichlet. In Figure 7.5 (right) we plot the real and imaginary part of $|u(x, 0.54)|^2$ for $V(x) = x^2$ and $\epsilon = 0.0256$. We include this example as a demonstration of the versatility of our 2D spectral method and are not arguing that it is computationally competitive to custom built methods such as those in [1].

**Example 5: The biharmonic equation.** The last example we consider is the biharmonic equation, a fourth order PDE, given by

$$u_{xxxx} + u_{yyyy} + 2u_{xxyy} = 0, \quad (x, y) \in [-1, 1]^2$$

with Dirichlet and Neumann boundary data corresponding to the function

$$v(x, y) = \text{Im} \left((x - iy)e^{-2(x + iy)} + \cos(\cos(x + iy))\right)$$

so that the solution is $u = v$. The implementation adaptively finds that a bivariate Chebyshev expansion of degree $(30, 30)$ is sufficient to resolve the solution to a maxi-
mum absolute error of \(4.59 \times 10^{-13}\) taking 2.52 seconds. This is a PDO with a splitting rank of 3 and hence the algorithm solves a large (but almost banded) linear system rather than a Sylvester matrix equation (see Section 6.1). When the underlying PDO has a splitting rank of \(k \geq 3\), the almost banded structure of ultraspherical spectral discretizations allows for fast linear algebra and hence, an \(O(\text{min}(n_x^3 n_y, n_x n_y^3))\) complexity of the solver.

8. Future work. The technique of automatic differentiation is far more powerful than we have described and could be extended to detect the linearity of a PDO or to compute a Fréchet derivative for solving nonlinear PDEs via Newton’s method in function space. For many years a similar approach has been employed in 1D to solve nonlinear ODEs in CHEBOP [6].

The spectral method we have described does, with some extra complications, extend to domains that can be decomposed into rectangles such as L-shaped domains. Such domains can be dealt with by solving coupled generalized Sylvester matrix equations with extra constraints imposing continuity of the solution. A significant challenge is to resolve potentially strong corner singularities in a solution that can result from intruding corners of the domain. General domains present a major challenge for global spectral methods.

We have presented a fast direct solver for PDOs with a splitting rank of 2, requiring \(O((n_x n_y)^{3/2})\) operations to compute a degree \((n_x, n_y)\) bivariate polynomial approximation. However, for PDOs with a splitting rank of \(k \geq 3\) we constructed a large almost banded matrix and solved the resulting linear system (see Section 6.1) in \(O(\text{min}(n_x^3 n_y, n_x n_y^3))\) operations. It would be interesting to investigate possible direct algorithms for solving generalized Sylvester matrix equations of the form (5.2) with \(k \geq 3\) terms.

Conclusion. We have described a spectral method for solving linear PDEs defined on rectangles. The first step was to extract the variable coefficients of a PDO from an anonymous operator using automatic differentiation. Then, by calculating a separable representation for the PDO we exploited the remarkable properties of the 1D ultraspherical spectral method to achieve a general, automated, and fast linear 2D PDE solver. The resulting 2D spectral method has a complexity of \(O(n_x^3 + n_y^3)\) for PDOs with a splitting rank of 2, when the solution is approximated by a bivariate polynomial of degree \(n_x\) in \(x\) and degree \(n_y\) in \(y\). The solver is part of CHEBFUN and is able to accurately solve a wide range of variable coefficient PDEs.

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